Study of localization effects in Falicov Kimball model: Dynamical Vertex Approximation

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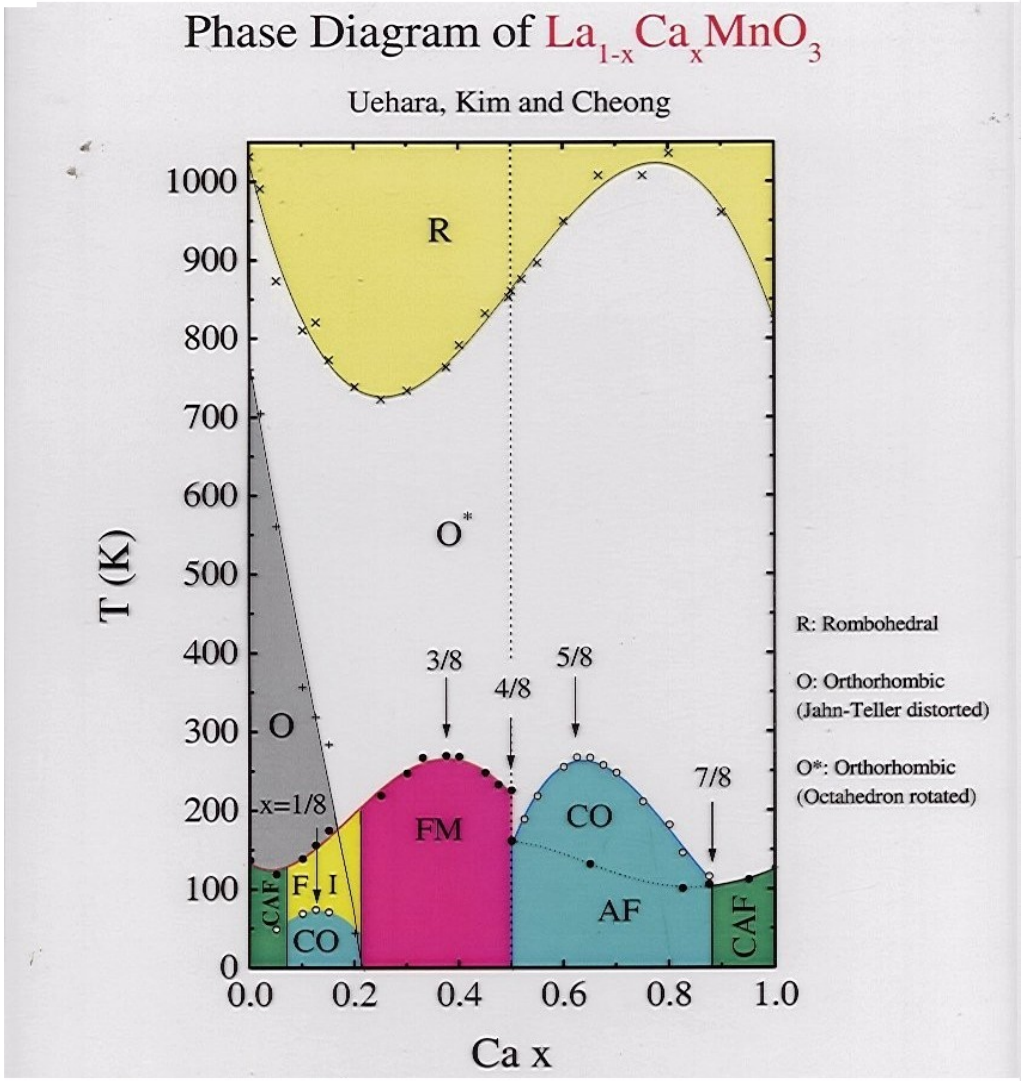
HOLE-DOPED MANGANITES: RICH VARIETY OF UNUSUAL PROPERTIES

- **Mix-valent oxides of Manganese**
- General formula : $A_{1-x}B_xMnO_3$
- A=Rare Earth element like La,Nd, Pr etc
  B= Alkaline Earth element like Sr, Ca etc
- **Rich phase diagram in Doping(x) – Temperature(T) plane:**
  Variety of phases:
  Ferromagnetic Insulator (FI)
  Ferromagnetic metal (FM)
  Paramagnetic Insulator (PI)
  Paramagnetic Metal (PM)
  Antiferromagnetic Insulator (AI)
  Charge, Orbital and
  Jahn-Teller ordered Insulator (COI)



PHYSICS OF MIT FROM L-B MODEL

- **Metal-Insulator Transitions as a function of both doping(x) and Temperature(T)**

- **Insultor→ Metal as x increases, or T decreases (since bandwidth increases)**

  - **As doping increases, number of *l* -polarons which can scatter mobile *b*-electrons reduces: hence bandwith increases.**

  - **As temperature decreases below T_c, spin-disorder decreases, hence less spin-dependent scattering, hence bandwidth increases.**

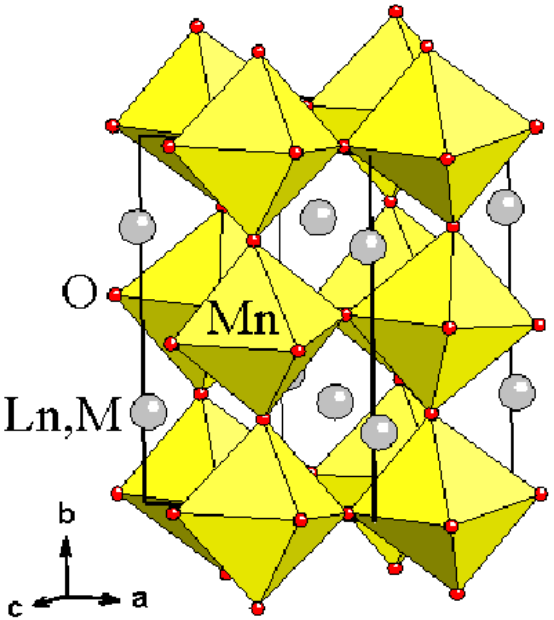
CRYSTAL CHEMISTRY OF MANGANITES

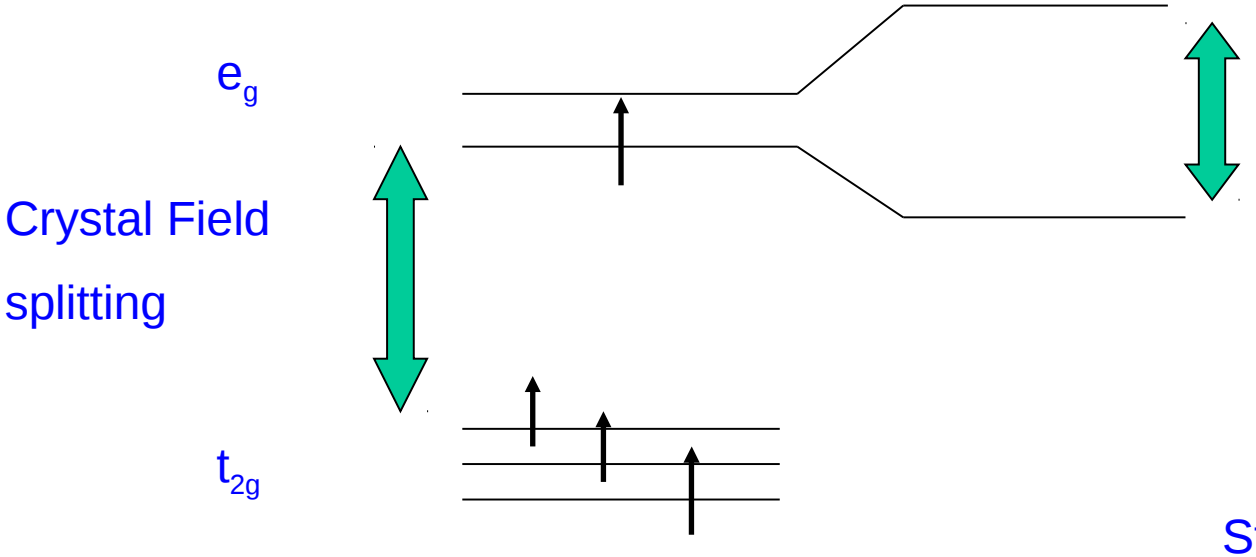
Manganites: $RE_{(1-x)}AE_xMnO_3$, eg. $La_{(1-x)}Ca_xMnO_3$

$LaMnO_3$: Mn^{3+} : $3d^4$ configuration

$CaMnO_3$: Mn^{4+} : $3d^3$ configuration

Hence, $La_{(1-x)}Ca_xMnO_3$: Mixed valency of Mn





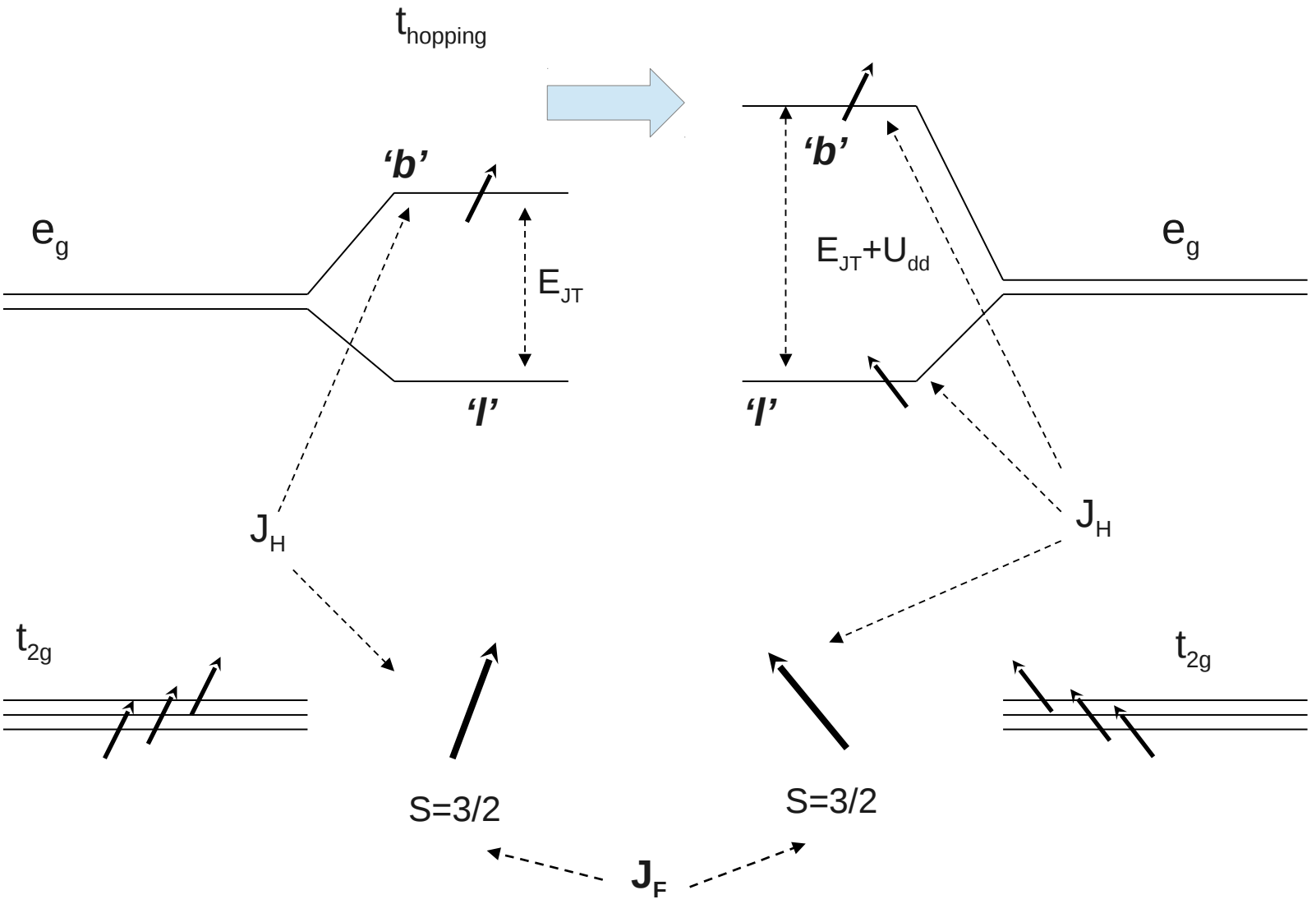
Jahn-Teller splitting

Strong Hund coupling!

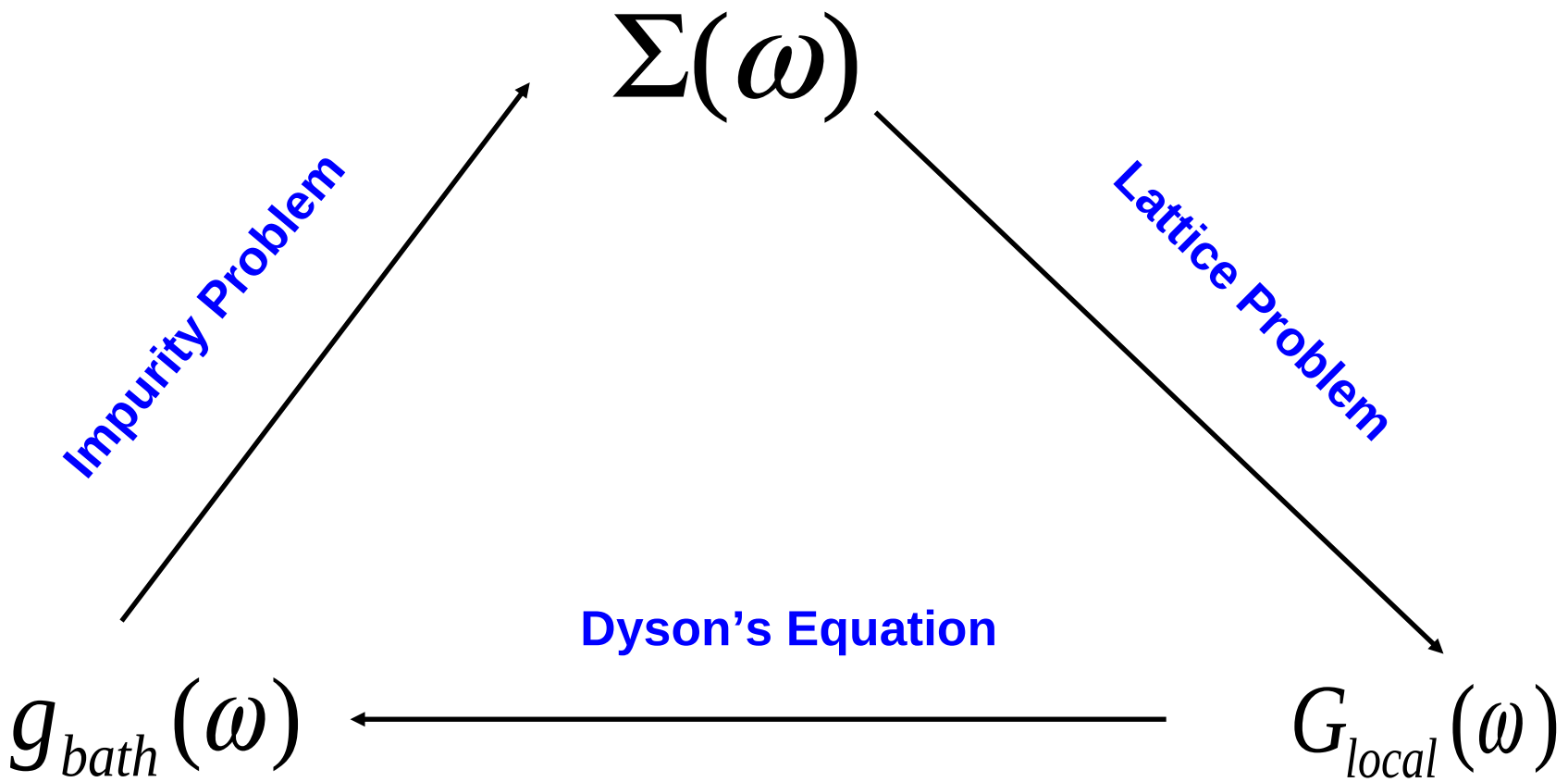
$LaMnO_3$

$CaMnO_3$

l-b model: schematic representation



DYNAMICAL MEAN FIELD THEORY

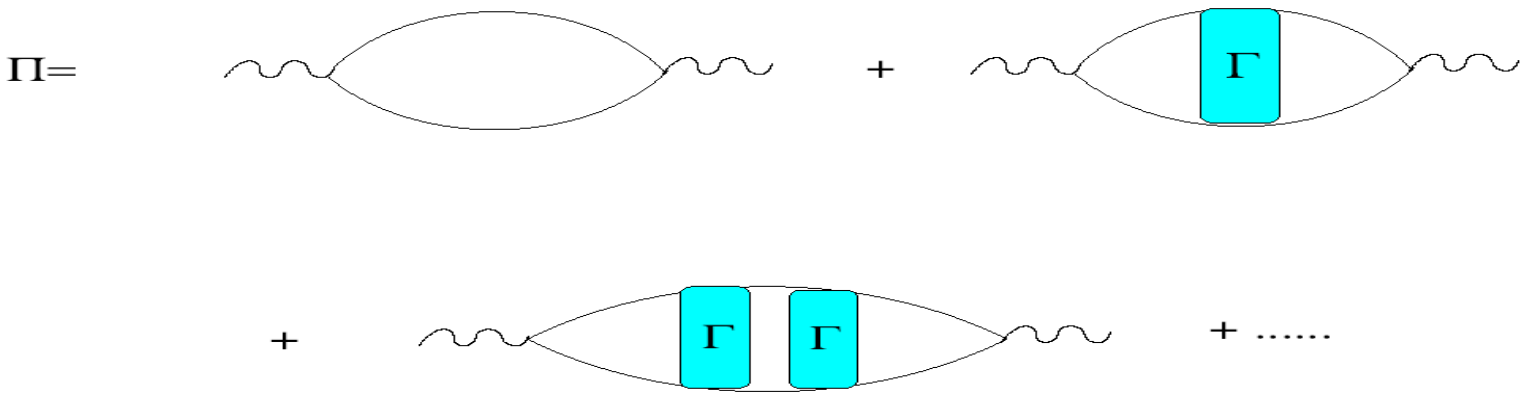


Calculate: Spectra, Conductivity, etc at finite T!

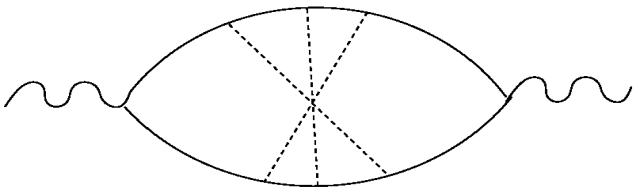
- Extrinsic disorder: Due to doping, defects, dislocations etc.: Not enough to produce significant localization in low-doping regime.

- **Intrinsic disorder due to immobile 'l' electrons: more efficient at producing localization, Anderson Insulator, Coulomb glass phases.**

• **TECHNICAL PROBLEM:** In the DMFT approximation, terms in the current-current correlation function Π in Kubo formula involving irreducible vertex parts Γ drop out.



• The important diagrams for Localization corrections to conductivity are maximally crossed diagrams, contained in the irreducible vertex parts.



• ***Hence, DMFT does not include Anderson Localization effects.*** To incorporate localization effects, we couple it with the **Self-consistent Theory of Localization.**

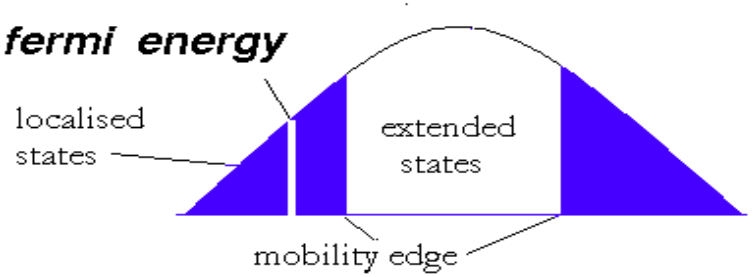
SELF-CONSISTENT THEORY OF LOCALIZATION (STL) AND THE POTENTIAL WELL ANALOGY (PWA)

- **Self-consistent theory of localization** gives a self-consistent relation for the full diffusion coefficient $D(\omega)$, or the full conductivity $\sigma(\omega)$, considering aforementioned maximally crossed diagrams.

- Formal analogy exists between this equation in the insulating phase for a **Localized State**, and the equation for a **Bound State** in a potential well in a tight-binding hypercubic lattice.

- **Since bound states can always appear for any arbitrary potential depth for dimensions d<3, hence, arbitrarily weak disorder can localize all states in one and two dimensions.**

- **In 3D, bound states can only occur beyond a critical well depth.** Similarly, localized states can only occur in certain energy windows. The energy separating extended and localized states is called **Mobility Edge.** The MIT occurs when the Fermi energy crosses the Mobility Edge.

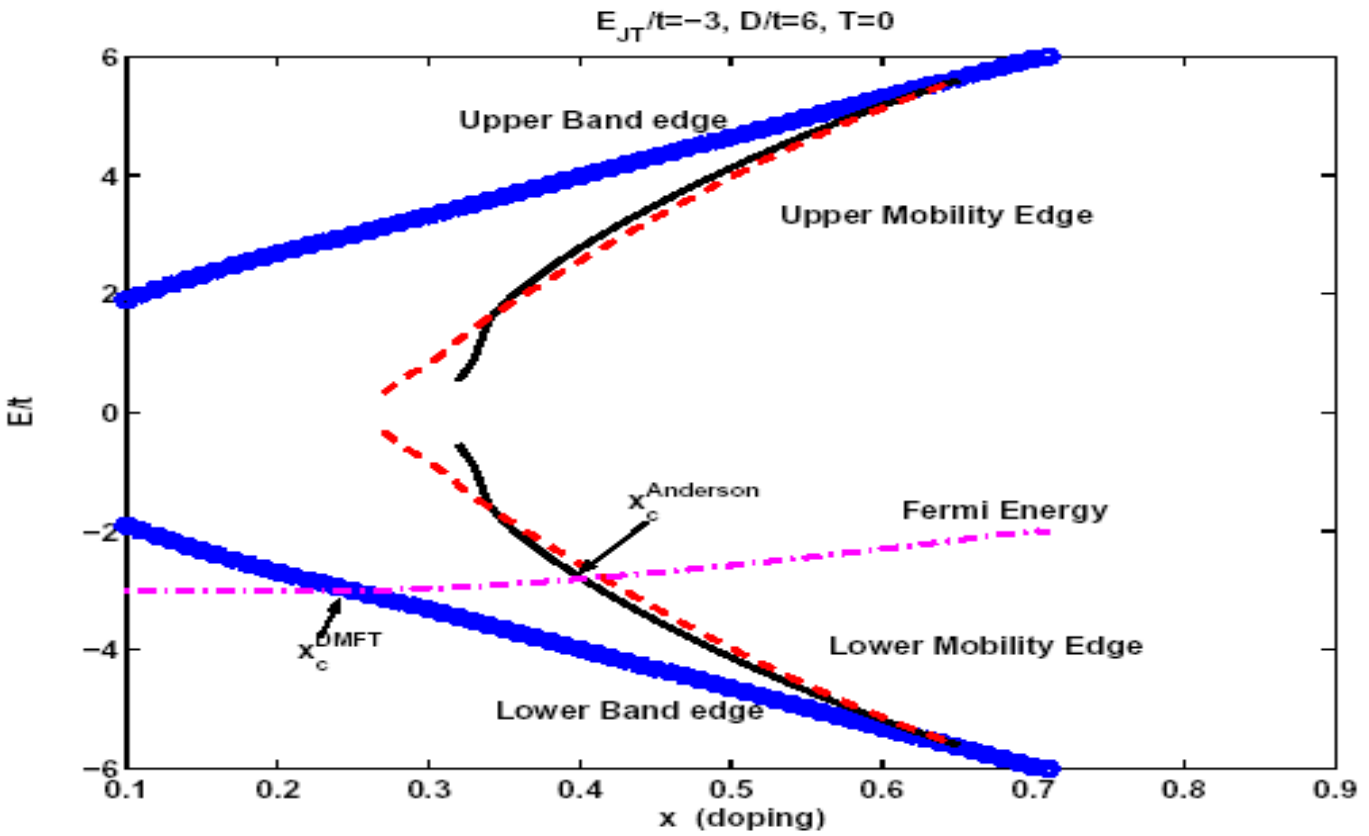


- The mobility edge trajectories diverge outwards from the band centre towards the band edges as the doping is increased.

- **Although the band bottom hits the local level at x=0.25, states at the Fermi energy are Anderson localized, giving rise to an Anderson Insulator phase.**

- **The actual MIT occurs only when the chemical potential meets the mobility edge, around x=0.4.**

- ***Chapter 1 of '50 Years of Anderson Localization' by E. Abrahams (World Scientific, 2010)***



Pair Susceptibility for maximally crossed diagrams

$$\chi(\tau) = \int_0^\beta d\tau \; Tr \frac{< e^{-\beta H} \Delta^d(\tau) \Delta^{d\dagger}(0) >}{Z_L} - \left[\frac{Tr < e^{-\beta H} \Delta^d >}{Z_L} \frac{< e^{-\beta H} \Delta^{d\dagger} >}{Z_L} \right]$$

The Auxilliary Green's function:

$$g^{aux}(\tau_1 \tau_2) = \frac{Tr T_\tau \left\langle e^{-\beta H_0} e^{\int_0^\beta \sum_p d\tau \chi_{1p}(\tau) \Delta(\tau)} d(\tau_1) d(\tau_2) \right\rangle}{1 + e^{\beta\mu \int_0^\beta d\tau \chi(\tau)}} + \frac{Tr T_\tau \left\langle e^{-\beta H_0} e^{\int_0^\beta d\tau \sum_p \chi^*_{1p}(\tau) \Delta^\dagger(\tau)} d^\dagger(\tau_1) d^\dagger(\tau_2) \right\rangle}{1 + e^{\beta\mu \int_0^\beta d\tau \chi(\tau)}}$$

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The local Green's function in DMFT:

$$G_{loc} = \frac{w_1}{\mathcal{G}^{-1} - U} + \frac{w_0}{\mathcal{G}^{-1}} \tag{1}$$

where $\mathcal{G}$=Wiess function in DMFT.

Dyson's equation:

$$G^{-1}(\omega) = \mathcal{G}^{-1}(\omega) - \Sigma \tag{2}$$

The dynamical vertex is obtained as:

$$\Gamma = \frac{\partial \Sigma}{\partial G} \tag{3}$$

Conclusion

We have calculated the dynamical vertex in the particle-particle channel from the pair susceptibility for the Falicov Kimball model.

Putting this along with the well known spin and charge vertex
In the parquet equation for the Dynamical Vertex Approximation, we can find the full irreducible vertex.

Using the Bethe Saltpeter equation, we can find the k-dependent self-energy from the irreducible vertex.

Then, putting back in the DMFT loop, one can get a self-consistency. Finally, one calculates the conductivity using the full Green's function and the vertex.