Transport and infrared optical response of ferromagnetic semiconductors: interplay between impurity scattering and dynamical many-body effects

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From Basic Concepts to Real Materials
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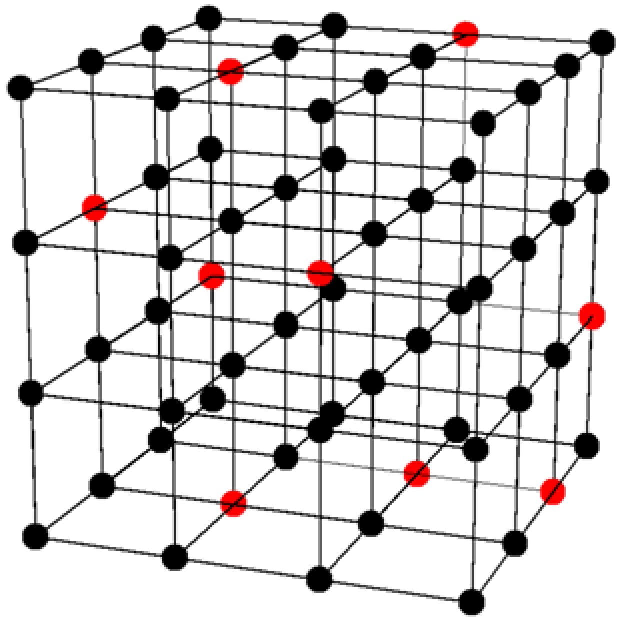
Outline

- Very Brief overview of DMS
- Theory of transport in spin & charge disordered media
- Temperature-dependent resistivity of GaMnAs
- Optical conductivity of GaMnAs: role of plasmons
- Correlated impurities

Diluted magnetic semiconductors (DMS)



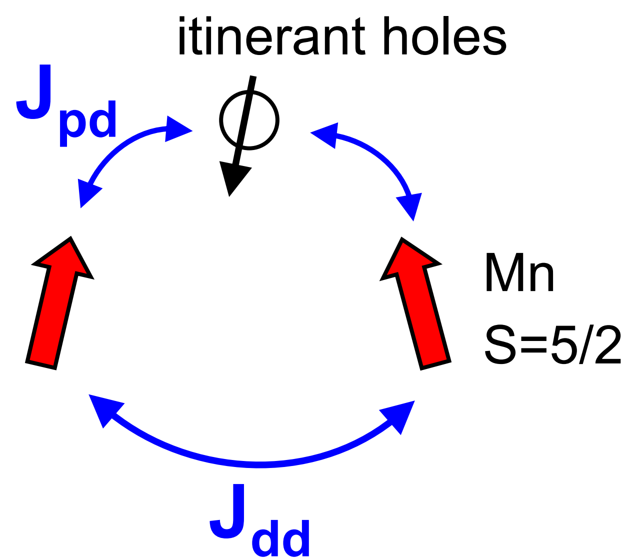
DMS: semiconductors with a small fraction of substituted magnetic ions

- ● III-V (GaAs, InAs, GaN)
  II-VI (CdTe, ZnSe, ZnO)
- ● Mn, Cr, Co, Fe

(Ga,Mn)As: Mn ions have localized spins, and are acceptors

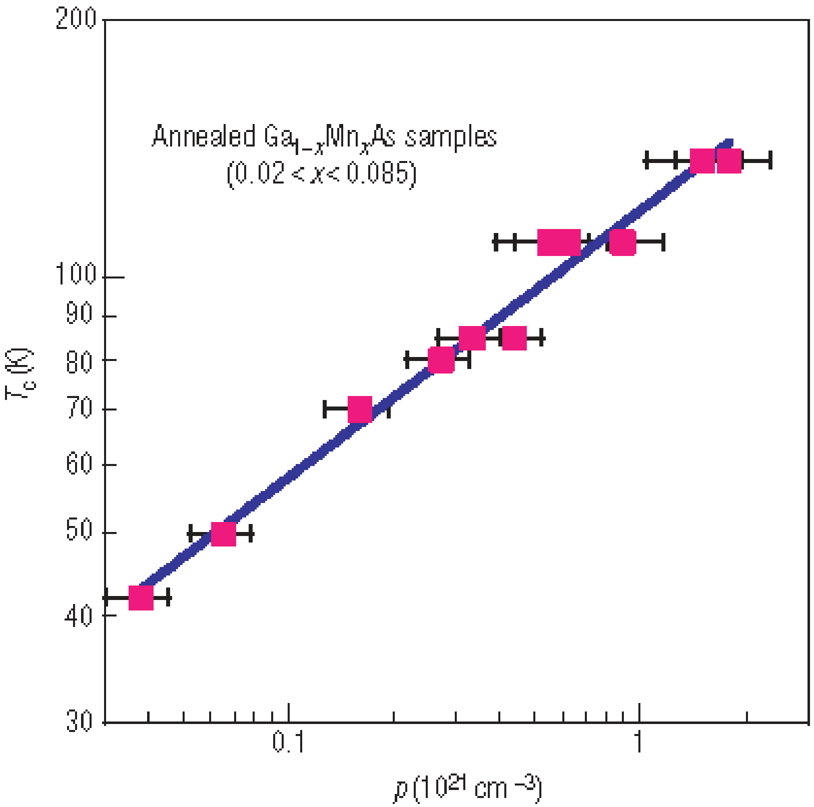
J_{dd}: AFM superexchange between local moments (small in III-V)

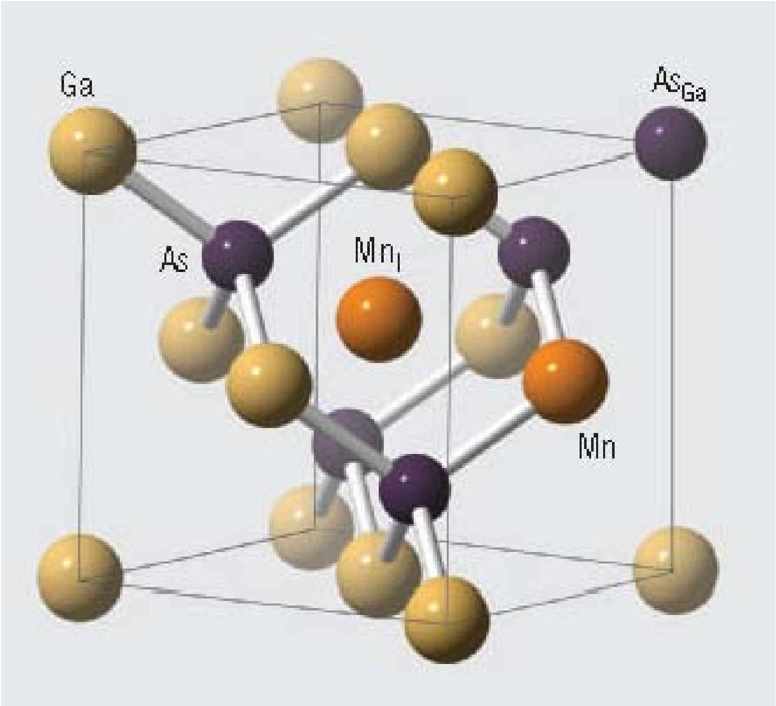
J_{pd}: AFM kinetic exchange between holes and local moments



(Ga,Mn)As: ferromagnetism and defects

A.H. MacDonald, P. Schiffer, and N. Samarth, Nature Mater. **4**, 195 (2005)
T. Jungwirth, J. Sinova, J. Masek, J. Kucera, and A.H. MacDonald, RMP **78**, 809 (2006)





- Ferromagnetism in (Ga,Mn)As for >2% Mn
- Increase solubility of Mn via low-temperature growth

As_{Ga} antisites
Mn_I interstitials
} double donors (compensation)

► Increase T_c by post-growth annealing (decrease # of Mn_I)

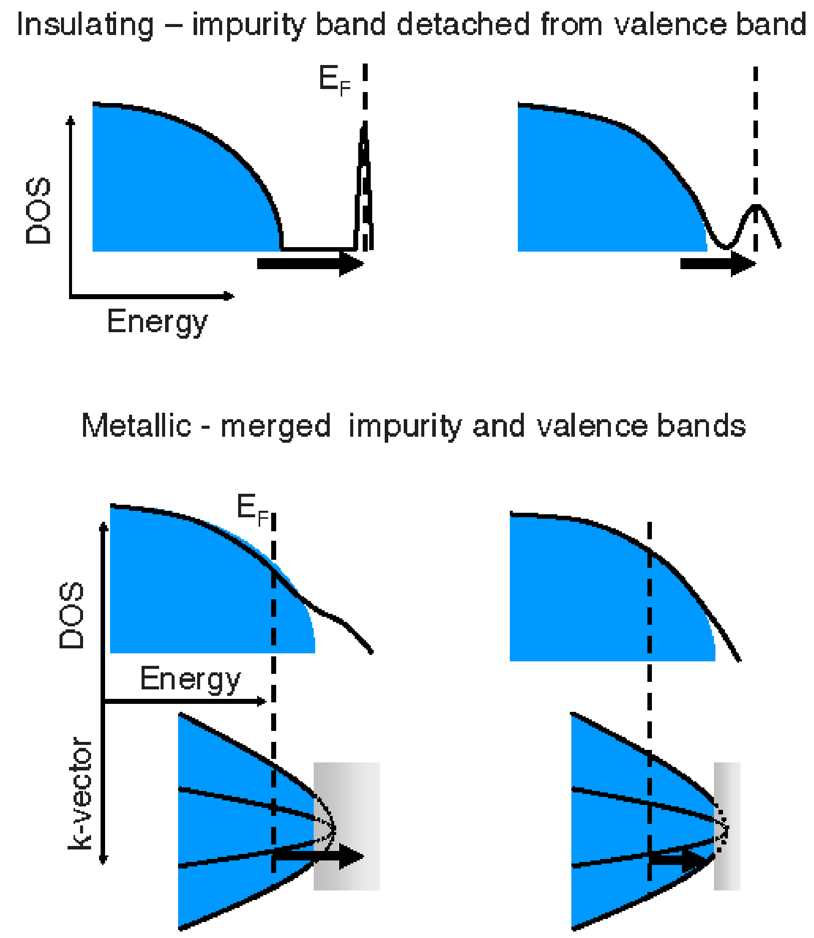
Itinerant carriers: valence vs impurity band

► **GaMnAs: some controversy**

- low doped insulating samples: carriers in impurity band
- heavier doped samples: possible valence band
- mixed messages from theory and experiment

► **Requirements for theory:**

- details of band structure
- Microscopic description of impurity scattering
- Electronic many-body effects (dynamical screening)



Jungwirth et al., PRB **76**, 125206 (2007)

Linear current response

$$\left\langle \hat{j}_\alpha(\mathbf{q},\omega)\right\rangle_{\mathbf{A}} = \sum_\beta \sum_{\mathbf{q}'} \left[\frac{n}{m}\delta_{\alpha\beta}\delta_{\mathbf{q}\mathbf{q}'} + \chi_{j_\alpha j_\beta}(\mathbf{q},\mathbf{q}',\omega)\right] \frac{e}{c} A_\beta(\mathbf{q}',\omega)$$

paramagnetic current-current response function:

$$\chi_{j_\alpha j_\beta}(\mathbf{r},\mathbf{r}',t) = -\frac{i}{\hbar}\Theta(t)\left\langle \left[\hat{j}_\alpha(\mathbf{r},t), \hat{j}_\beta(\mathbf{r}')\right]\right\rangle_{\hat{H}}$$

► We consider the spin-independent response to a spin-independent perturbation in a spin-dependent medium.

► Calculate χ_{jj} in the presence of charge and magnetic disorder, using equation of motion approach.

Total system Hamiltonian

$$\hat{H} = \hat{H}_e + \hat{H}_m + \hat{H}_d$$

clean-system part:

$\hat{H}_e$: itinerant carriers (8-band **k•p**)

$\hat{H}_m$: subsystem of localized magnetic spins (mean-field)

disorder part:

$$\hat{H}_d = V^2 \sum_{\mathbf{k}} \hat{\vec{U}}(\mathbf{k}) \hat{\vec{\rho}}(-\mathbf{k})$$

charge and spin disorder scattering

4-component density operator

$$\hat{\vec{\rho}} = \begin{pmatrix} \hat{n} \\ \hat{s}^+ \\ \hat{s}^- \\ \hat{s}^z \end{pmatrix}$$

Disorder scattering potential

$$\hat{\vec{U}}(\mathbf{k}) = \frac{1}{V}\sum_j \begin{pmatrix} U_j(\mathbf{k}) \\ -(J/2)\hat{S}_j^- \\ -(J/2)\hat{S}_j^+ \\ -(J/2)\left(\hat{S}_j^z - \langle S \rangle\right) \end{pmatrix}$$

- ► Can have multiple types of defects. Most important: Mn_{Ga}
- ► Defects can be randomly distributed or correlated
- ► Spin disorder: fluctuations of localized spins around mean-field value.

Current response in the presence of disorder

$$\chi^{J}_{\alpha\beta}(\mathbf{q},\omega) = \chi^{\mathbf{C}}_{j_{p\alpha} j_{p\beta}}(\mathbf{q},\omega) + \frac{n}{n}\delta_{\alpha\beta}$$

$$+\frac{V^2}{m^2\omega^2}\sum_{\substack{\vec{k}\\ \mu\nu}} k_\alpha k_\beta \left\langle \hat{U}_\mu(\mathbf{k})\hat{U}_\nu(-\mathbf{k})\right\rangle_{\hat{H}_m} \left\{\chi^{\mathbf{C}}_{\rho_\mu\rho_\nu}(\mathbf{q}-\mathbf{k},\omega) - \chi^{\mathbf{C}}_{\rho_\mu\rho_\nu}(-\mathbf{k},0)\right\}$$

weak-disorder limit

self-consistency via continuity equations
→can go to strong disorder limit

- ►Follows from equation of motion and decoupling of Force-Force correlation function
- ► $\chi^{\mathbf{C}}$ contains electronic many-body effects (screening etc.), in principle exactly via **TDDFT**
- ► Additional terms resulting from noncommuting components of $\hat{\vec{U}}$ vanish in the paramagnetic limit (but not in FM case)

Relaxation rates for charge and spin scattering

Drude expression in weak disorder limit $\omega\tau >> 1$:

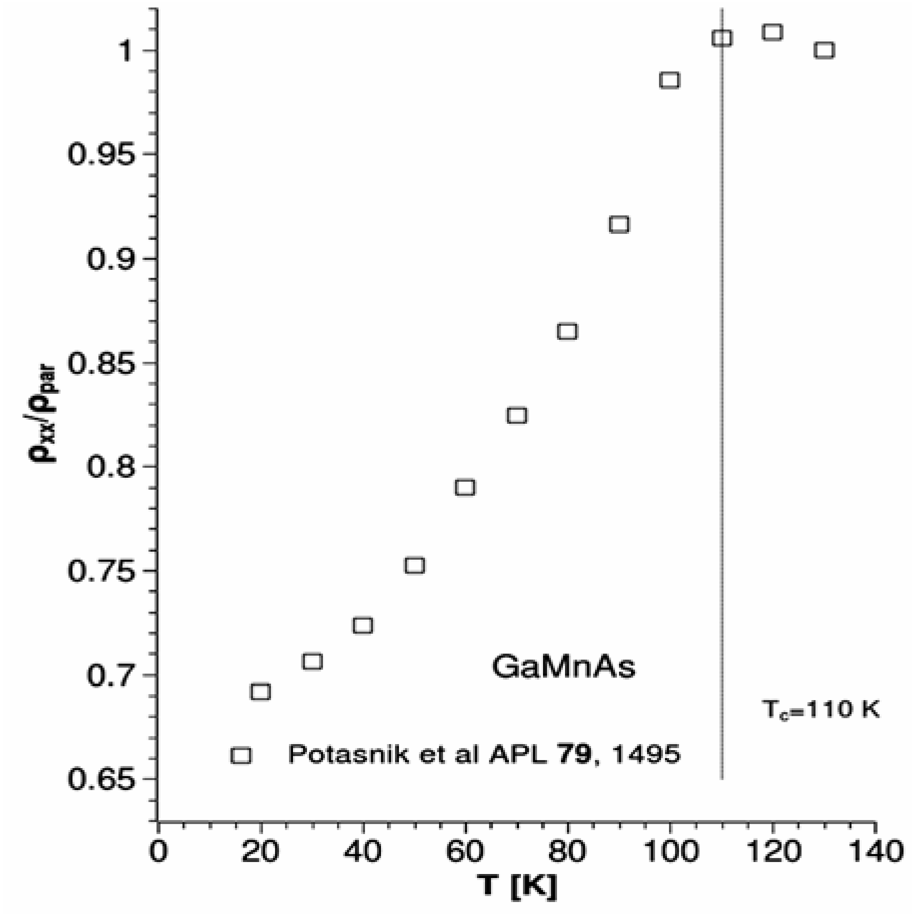
$$\chi_D^J(\omega) = \frac{n}{m}\frac{1}{1+(\omega\tau)^{-1}} \approx \frac{n}{m} - \frac{n}{m\omega}\frac{1}{\tau}$$

$$\tau_{\alpha\beta}^{-1}(\mathbf{q},\omega) = i\frac{V^2}{nm\omega}\sum_{\mathbf{k},\mu\nu} k_\alpha k_\beta \left\langle \hat{U}_\mu(-\mathbf{k})\hat{U}_\nu(\mathbf{k})\right\rangle_{H_m} \times\left[\chi_{\rho^\mu\rho^\nu}(\mathbf{q}-\mathbf{k},\omega) - \chi_{\rho^\mu\rho^\nu}(\mathbf{k},0)\right]$$

TDDFT: $$\chi^{-1}(\mathbf{q},\omega) = \chi_0^{-1}(\mathbf{q},\omega) - v(\mathbf{q}) - f_{xc}(\mathbf{q},\omega)$$

8-band **k•p** ALDA

Temperature dependence of static resistivity



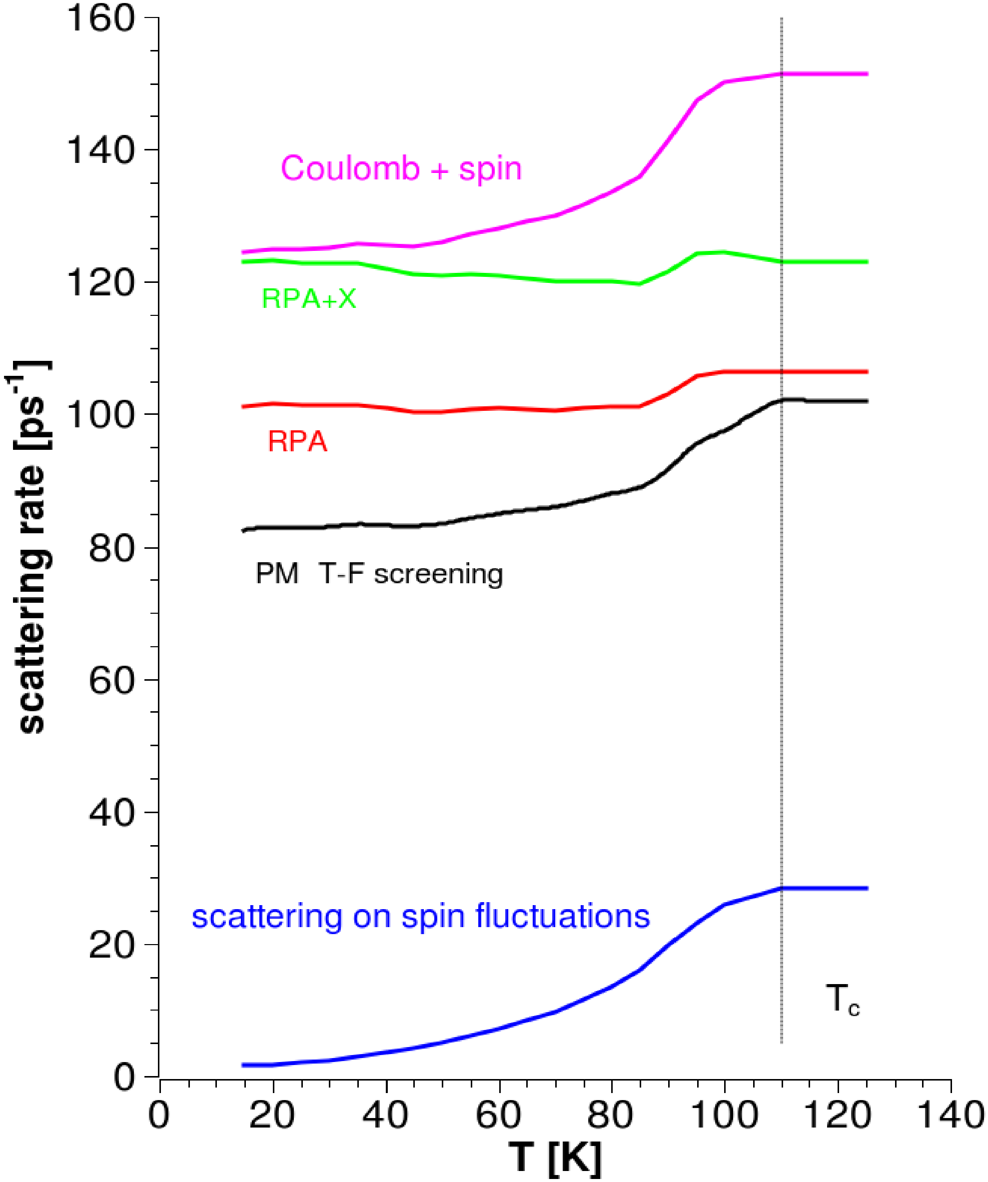
► Pronounced drop in resistivity below ferromagnetic T_c

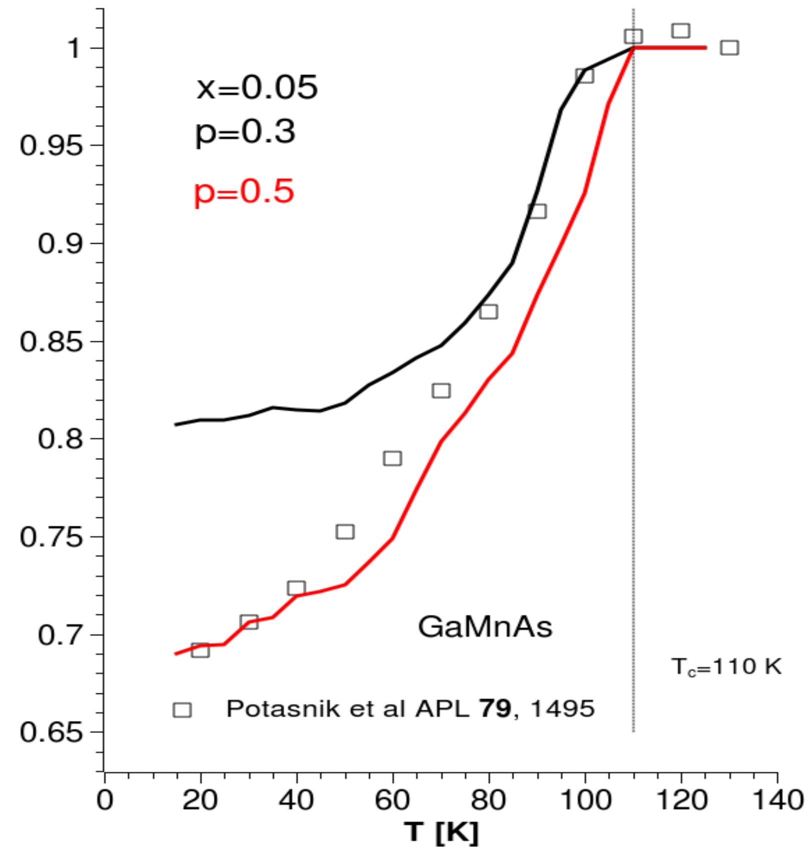
► Previous theoretical work:

- Only Coulomb disorder
- Only static screening
- Attributed to changes of the Fermi surface due to the FM transition

[Lopez-Sancho and Brey, PRB **68**, 113201 (2003)]

Temperature dependence of static resistivity

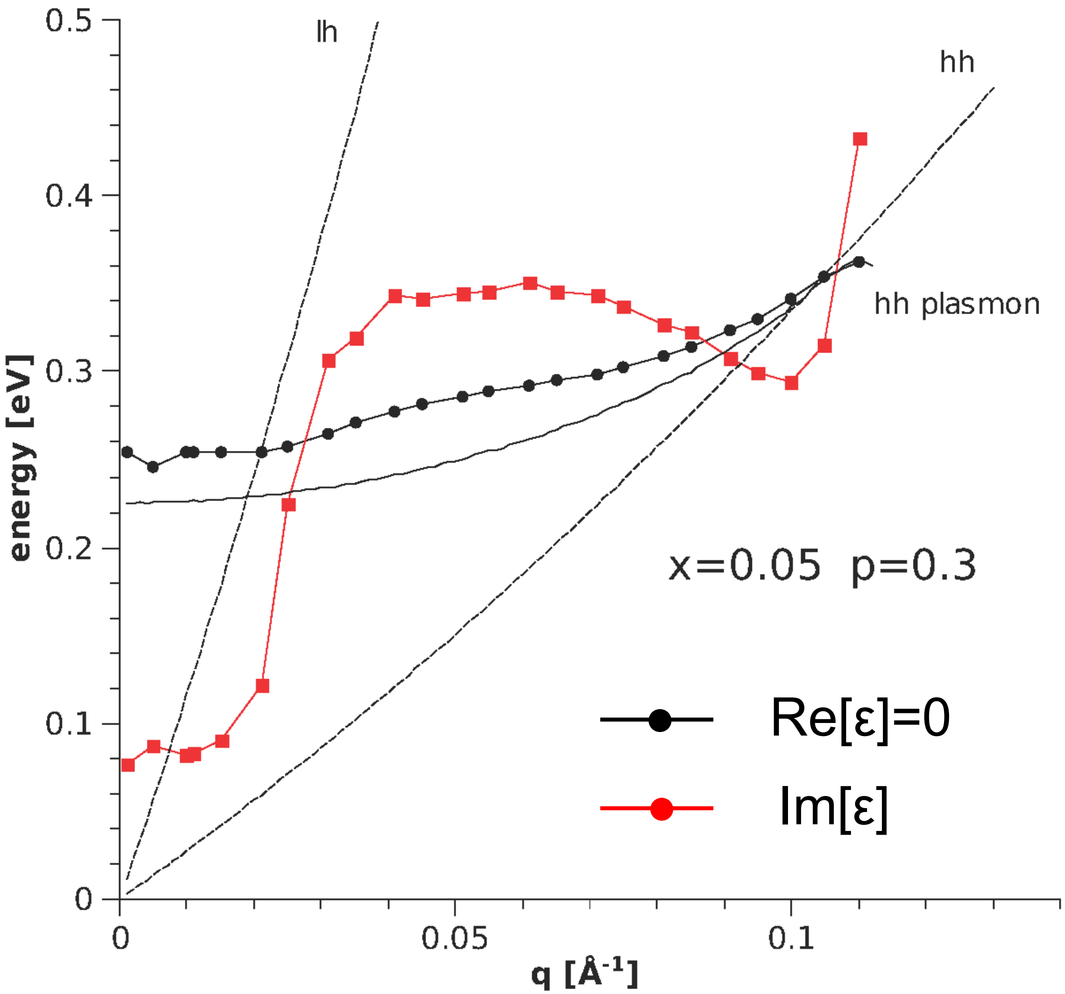


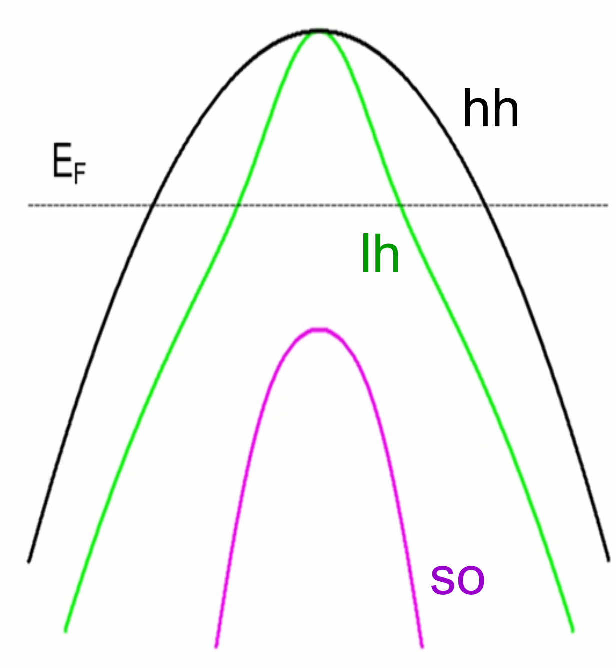


F.V. Kyrychenko and C.A.U. PRB **80** (2009), in press

Resistivity drop due to the suppression of the scattering off localized spin fluctuations

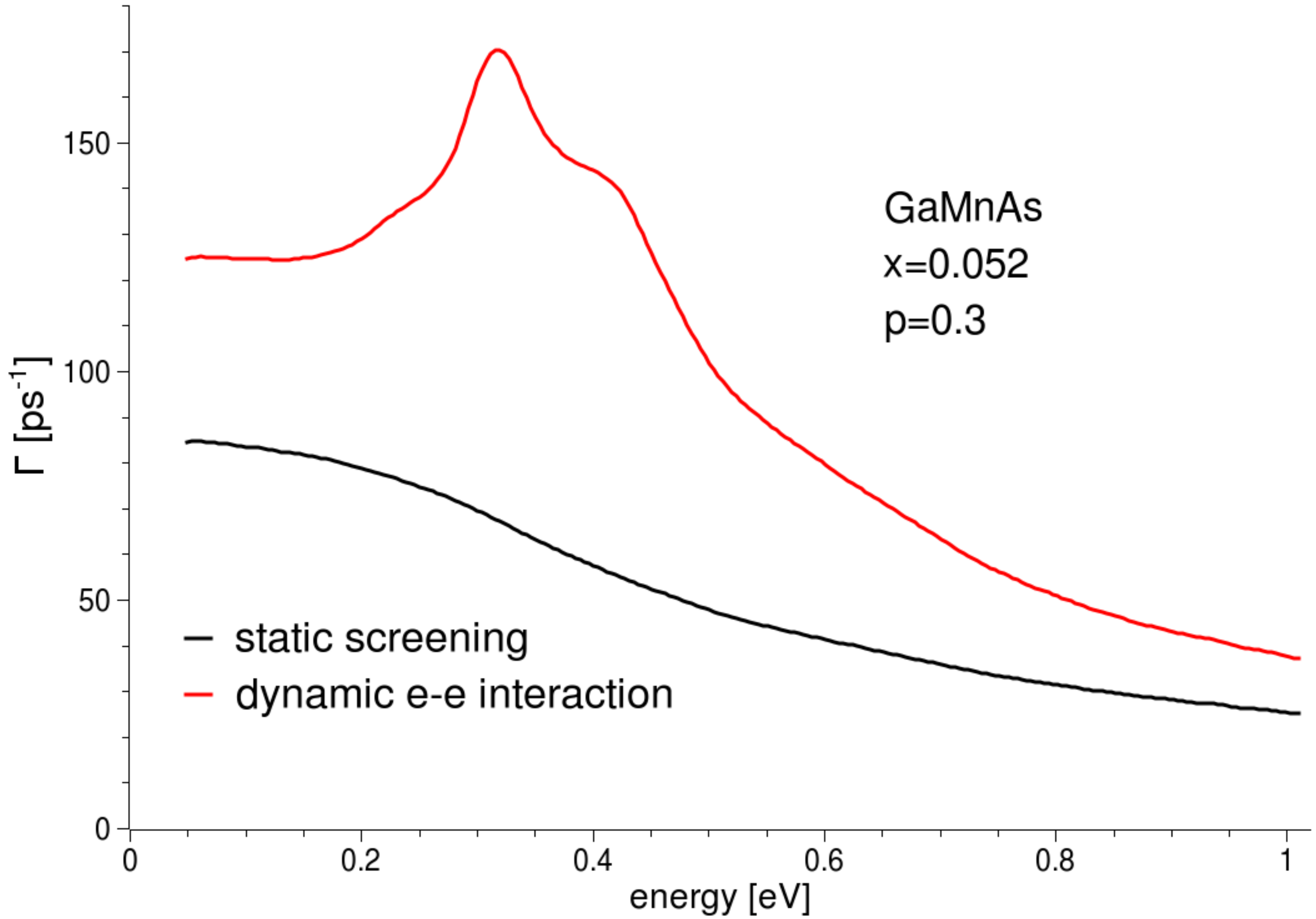
Dynamical screening and valence band plasmons



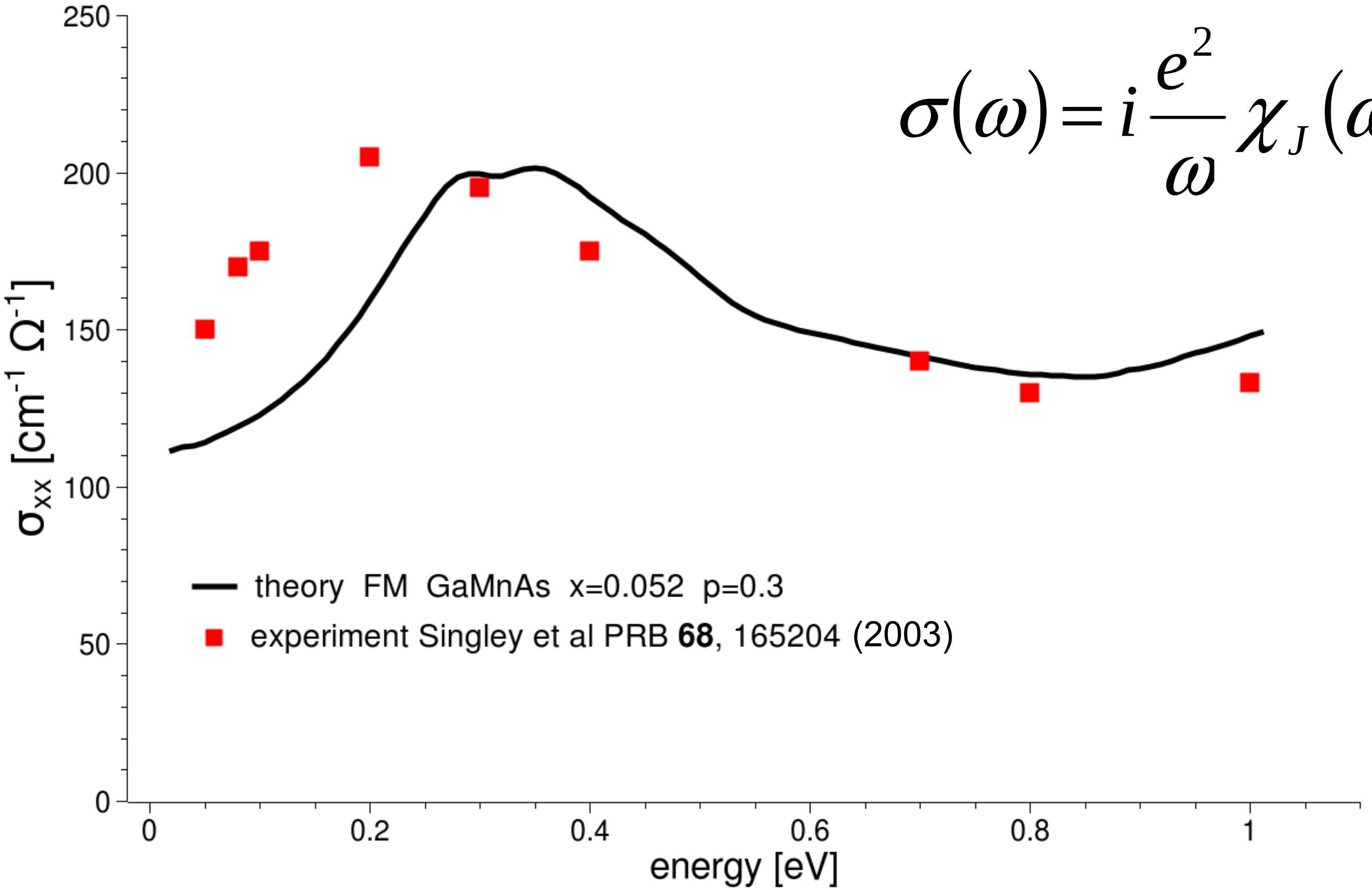


- Plasmons in p-type semiconductors are strongly damped
- Damping due to coupling with inter- and intra-valence band continua

Static vs dynamic screening



Infrared conductivity

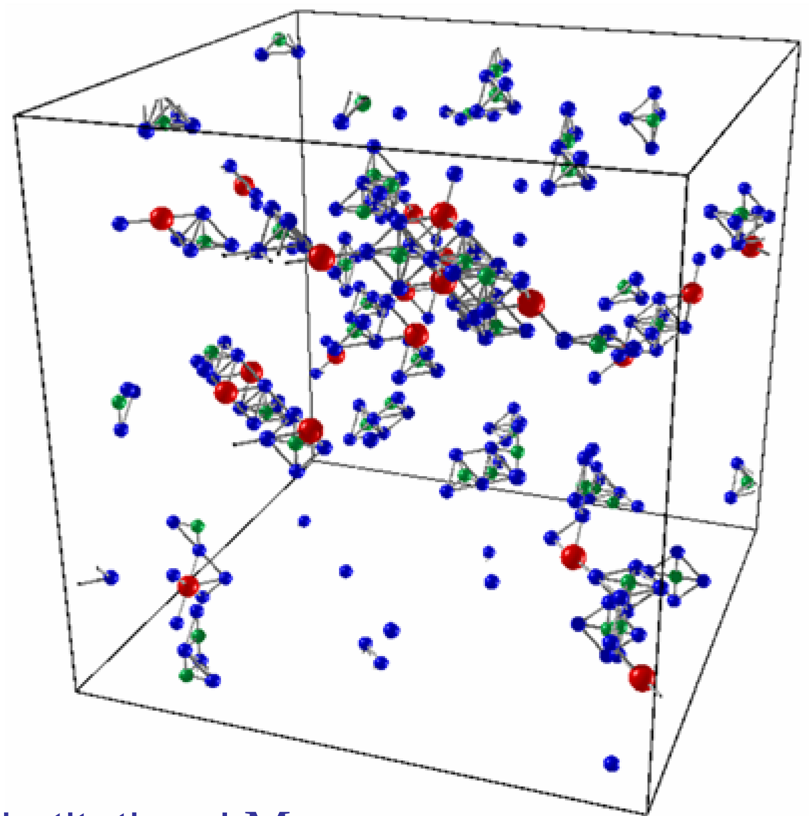


$$\sigma(\omega) = i\frac{e^2}{\omega}\chi_J(\omega)$$

- Optical conductivity dominated by inter-valence band transitions
- Broadening strongly frequency-dependent
- No impurity band involved ⟺ Hankiewicz et al, PRB **70**, 245211 (2004)

(Ga,Mn)As: correlations in defect positions

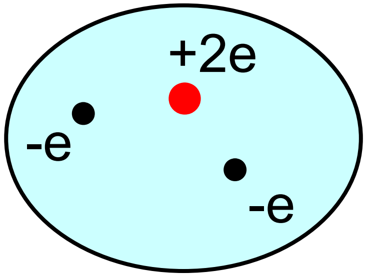
C. Timm, F. Schäfer, and F. von Oppen, PRL **89**, 137201 (2002)
C. Timm, J. Phys.: C. M. **15**, R1865 (2003)



● substitutional Mn_{Ga}
● antisites As_{Ga}
● Mn-interstitials

Monte Carlo equilibrium configuration

► Defect correlation through Coulomb interaction



ionic screening

► explains experimental trends:
- mobility edge vs. doping
- magnetization M(T) more mean-field like

► may enhance Curie temp.

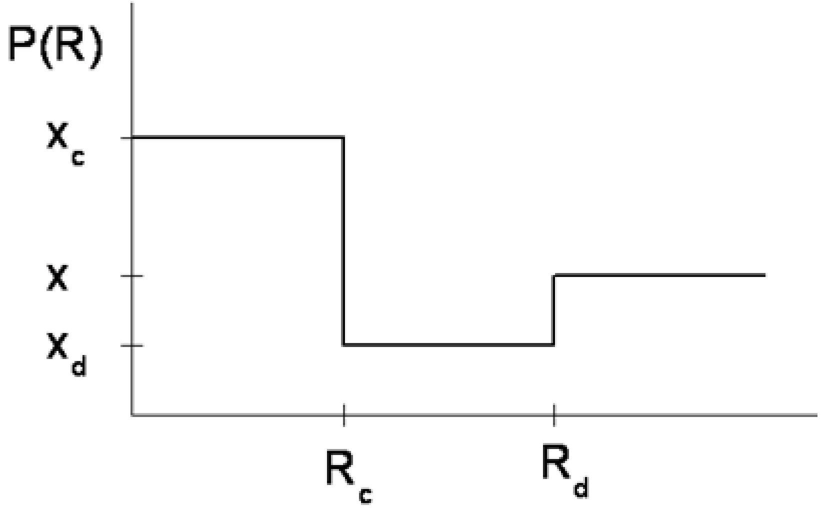
G. Bouzerar, T. Ziman, and J. Kudrnovsky, APL **85**, 4941 (2004)

(From http://www.people.ku.edu/~ctimm/Hess.html)

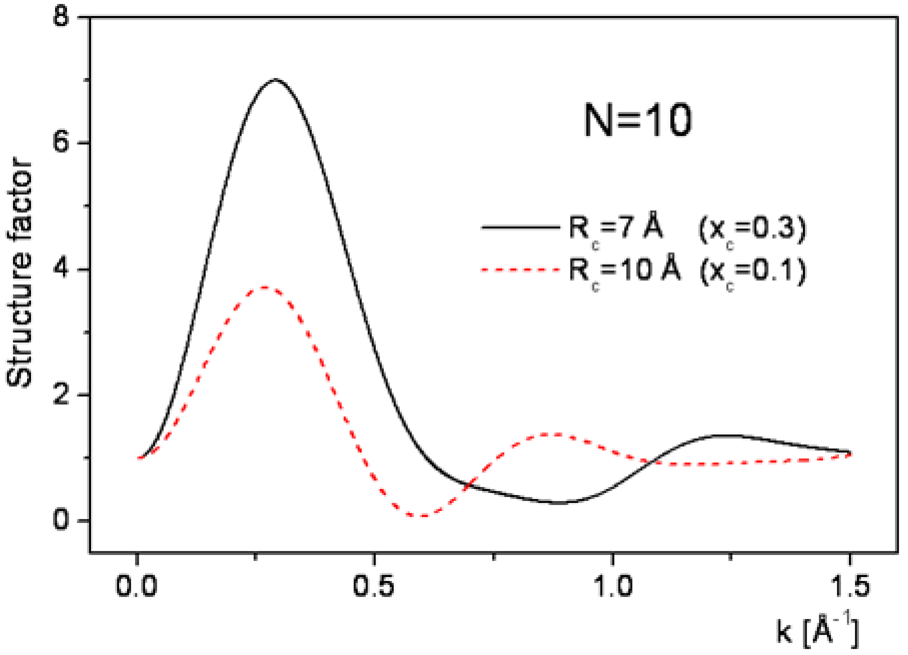
Model for correlated charge disorder

$$\left\langle \hat{U}_n(\mathbf{k})\hat{U}_n(-\mathbf{k})\right\rangle = \left|U_n(\mathbf{k})\right|^2 \frac{n_i}{V} S(\mathbf{k})$$

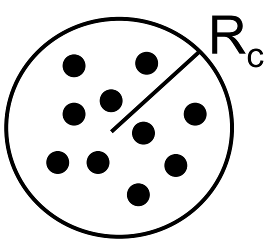
pair distribution function:



structure factor:

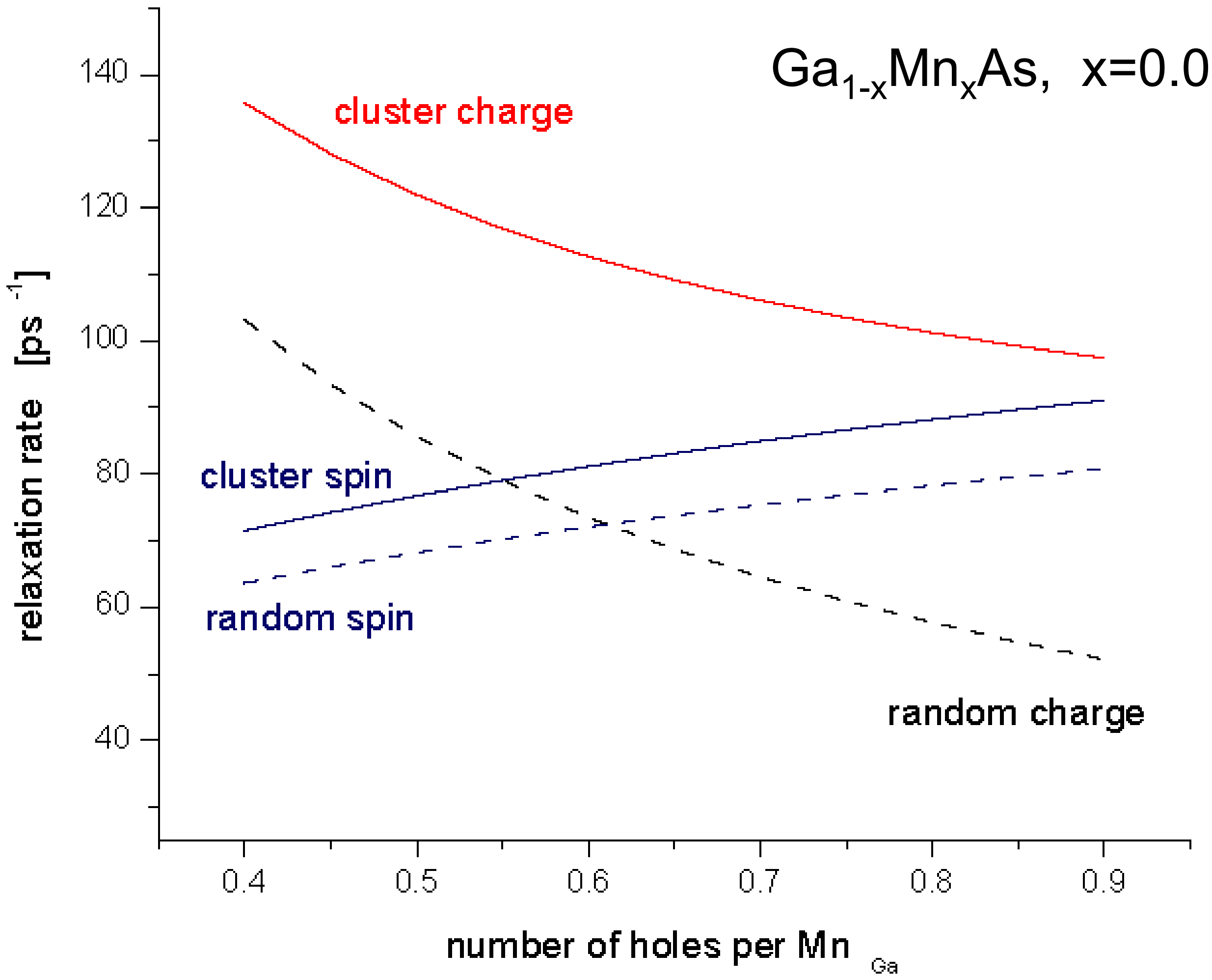


N=10 (average # of Mn ions in a "cluster")



$$S(\mathbf{k}) = 1 + \int P(\mathbf{R})\cos(\mathbf{k}\cdot\mathbf{R})\, d\vec{R}$$

Relaxation rates (paramagnetic regime)



50-100% enhanced relaxation rate

F.V. Kyrychenko and C.A. Ullrich, Phys. Rev. B **75**, 045205 (2007)

Acknowledgments

Group:

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- Klaus Capelle (Sao Carlos/Brazil)
- Giovanni Vignale (MU)
- Volodymyr Turkowski (UCF)

Summary

- **Theory of transport and optical conductivity in DMS:**
  - ► self-consistent → works for weak and strong disorder
  - ► can describe random or correlated disorder, charge and spin
  - ► combine with TDDFT → dynamic many-body effects

- **Application to (GaMn)As:**
  - ► Temperature-dependent resistivity
  - ► Optical conductivity
  - ► Supports the valence band picture for x~3-5% Mn doping

F.V. Kyrychenko and C.A. Ullrich, Phys. Rev. B **75**, 045205 (2007)
F.V. Kyrychenko and C.A. Ullrich, J. Phys.: Cond. Mat. **21**, 084202 (2009)
F.V. Kyrychenko and C.A. Ullrich, Phys. Rev. **80** (2009), in press