A Heisenberg model for describing the magnetic properties of GaMnAs. Study of thermal and quantum fluctuations.

cond-mat/0306125

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A DESCRIPTION OF THE MAGNETIC PROPERTIES OF DMS BASED JUST ON THE POSITIONS AND SPIN ORIENTATION OF THE Mn's .

Heisenberg like Hamiltonian.

$$E = E_{KE} + \sum_{I,J} J_{I,J}(R_{I,J})\, \vec{S}_I \cdot \vec{S}_J$$

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- Realistic band structure

BEYOND MEAN FIELD APPROXIMATION.

- Thermal fluctuations.
- Disorder effects.
- Quantum fluctuations.
- **Is it the T=0 ground state collinear?**

H=H$_0$+ΔV

$$H = H^{\vec{k}\cdot\vec{p}}_{holes} + \underbrace{\sum_{I,i} \vec{S}_I \cdot \vec{s}_i \, J(\vec{R}_I - \vec{r}_i)}_{\Delta V}$$

- **Mn have S=5/2.**
- **Mn are diluted and do not interact directly.**
- **Strong -AF- coupling between Mn spins and hole spins.**

$$J(\vec{r}) = \frac{J_{pd}}{(2\pi a_0)^{3/2}} e^{-r^2/2a_0^2}$$

$$< n\vec{k} \,|\, \Delta V \,|\, n'\vec{k}' >= \frac{V\, J_{pd}}{N^2} \sum_I \alpha^{J,m_J}_{n,\vec{k}} \alpha^{J',m'_J}_{n',\vec{k}'} \; \vec{s}_{Jm_J,J'm'_J} \cdot \vec{S}_I \; e^{-i(\vec{k}'-\vec{k})\vec{R}_I} \; e^{-|\vec{k}-\vec{k}'|^2 \frac{a_0^2}{2}} (1-\delta_{\vec{k},\vec{k}'}$$

Justification of the model.

$$E = E_{KE} + \sum_{I,J} J_{I,J}(R_{I,J})\, \vec{S}_I \cdot \vec{S}_J$$

Pairwise interaction for Mn spins (exact results)

1. **k·p** Luttinger Hamiltonian. Anisotropy in the spin interactions.

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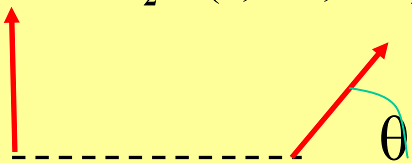
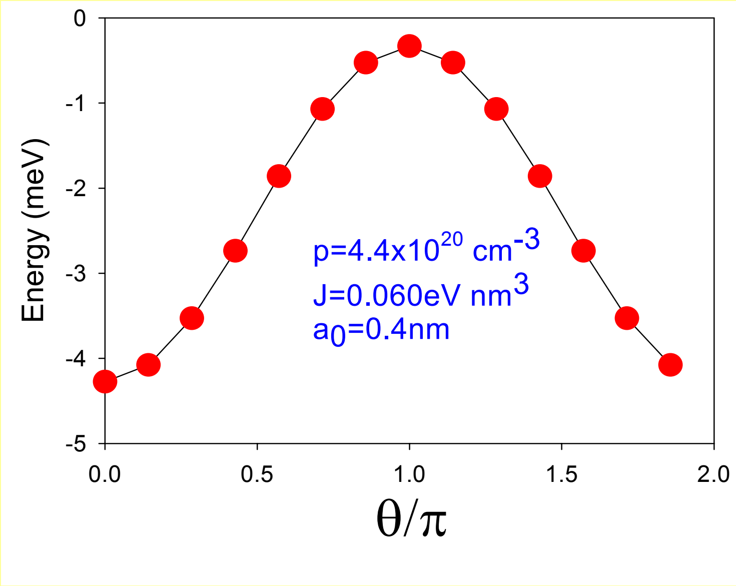
$\mathbf{S_1}$=S(0,0,1)
$\mathbf{S_2}$=S(0,sinθ,cosθ)

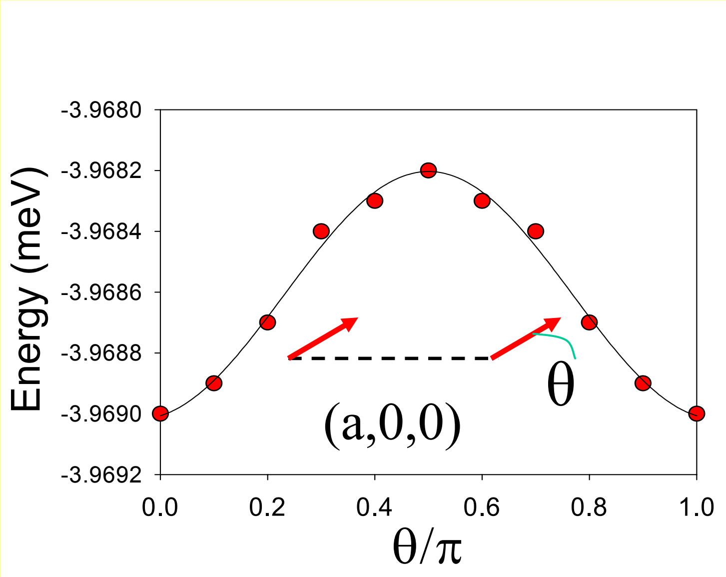


wo spins located in (000) and (1,1,0)a/2.



$\vec{S}_1 \cdot \vec{S}_2$

Zarand and Janko PRL'02



$\mathbf{S_2}$=$\mathbf{S_1}$=S(0,sinθ,cosθ)

The interaction between Mn spin is almost isotropic and fit very well with a $\mathbf{S_I}$·$\mathbf{S_J}$ term.

E_1

E_2

	E_1	E_2
4band	-2.12	-1.65
6band (a_0=0)	-4.45	-4.26
6band (a_0=0.4nm)	-2.04	-2.03

Pairwise interaction for Mn spins (exact results)

. **k·p** Luttinger Hamiltonian. Anisotropy in the spin interactions.

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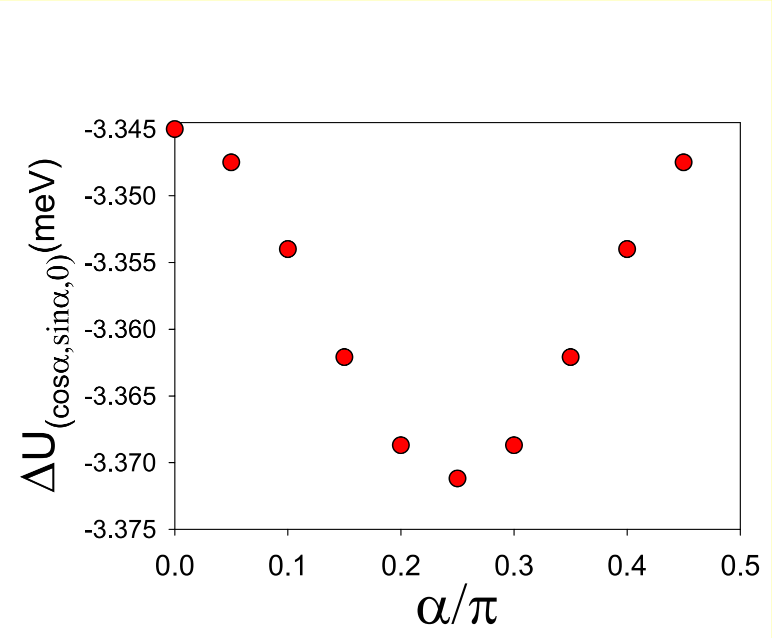
2. **k·p** Luttinger Hamiltonian has cubic symmetry. [001], [111], [110] not equivalents



2 Mn spins pointing in the z-direction
And separated by a vector (cosα,sinα,0).

Isotropy in the magnetization orientation is a good approximation

Pairwise interaction for Mn spins (exact results)

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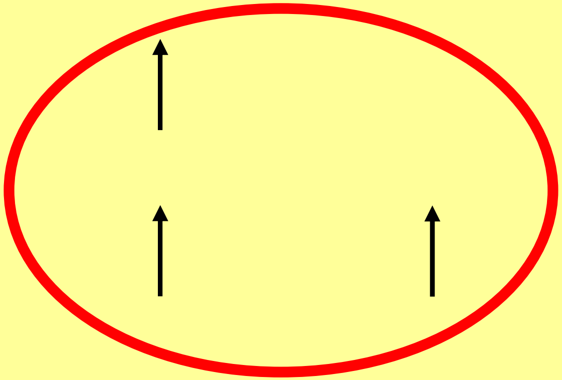
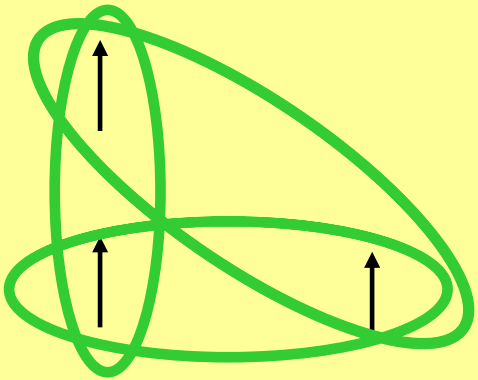
3. Virial expansion.

The energy of a system of three Mn spins located on the positions (0,0,0), (a,0,0) and (0,a,0), can be expressed as the sum of pair interactions plus self-energies. (5.043meV versus 5.031 meV).





Pairwise interaction for Mn spins (exact results)

1. **k·p** Luttinger Hamiltonian. Anisotropy in the spin interactions.

   The interaction between Mn spin is almost isotropic and fit very well with a $S_I S_J$ term.

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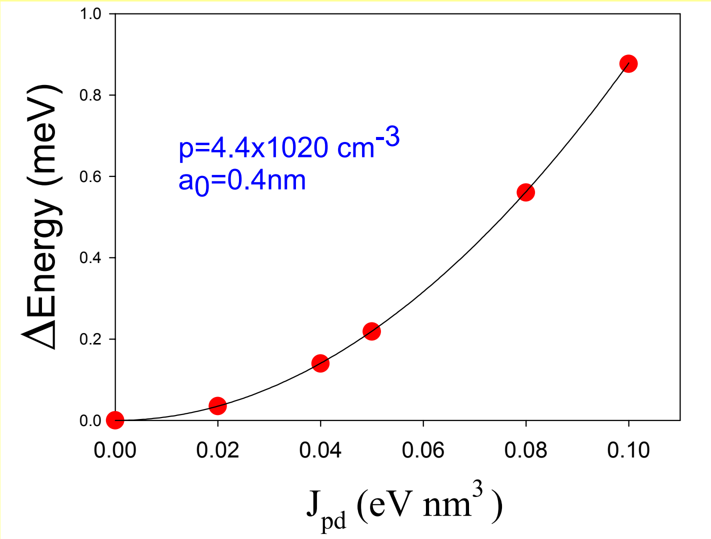
   Isotropy in the magnetization orientation is a good approximation

3. Virial expansion.

4. For J_{pd} smaller than 0.10eV nm^3 the interaction energy is quadratic in J_{pd}.



$$\Delta\text{Energy}=(E_{\parallel} - E_{\perp})/2$$

Perturbation theory is valid.

Heisenberg like Hamiltonian.

$$H = \sum J_{I,J}(R_{I,J})\,\vec{S}_I \cdot \vec{S}_J$$

$$J(\vec{R}_{IJ}) = -\frac{1}{N}\sum j(\vec{q})e^{i\vec{q}\vec{R}_{IJ}}$$

$$j(\vec{q}) = J_{pd}^2 \frac{N}{\Omega}\chi_p(\vec{q})e^{-q^2 a_0^2}$$

p=0.05-0.6 nm^{-3}

J_{pd} up to 0.13eVnm^3

Different Curie Temperatures...

$$H = \sum J_{I,J}(R_{I,J})\,\vec{S}_I \cdot \vec{S}_J$$

$$k_B T_C^{mf} = \frac{S^2}{3} x \sum_{I \neq 0} J(R_I) = k_B T_C^{vca} \left(1 - \frac{1}{N} \sum_q \frac{\chi_p(q) e^{-q^2 a_0^2}}{\chi_p(q=0)} \right)$$

Ginsburg criterion T*

$$\left(m(T^*)\right)^2 = G < m^2 >_{T_C^{mf}}$$

Monte Carlo T_C

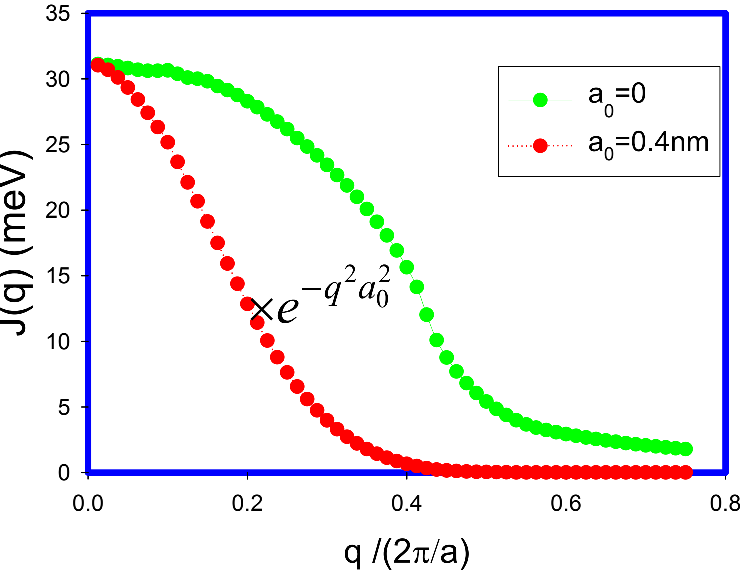
Effect of thermal fluctuations and disorder on T_c

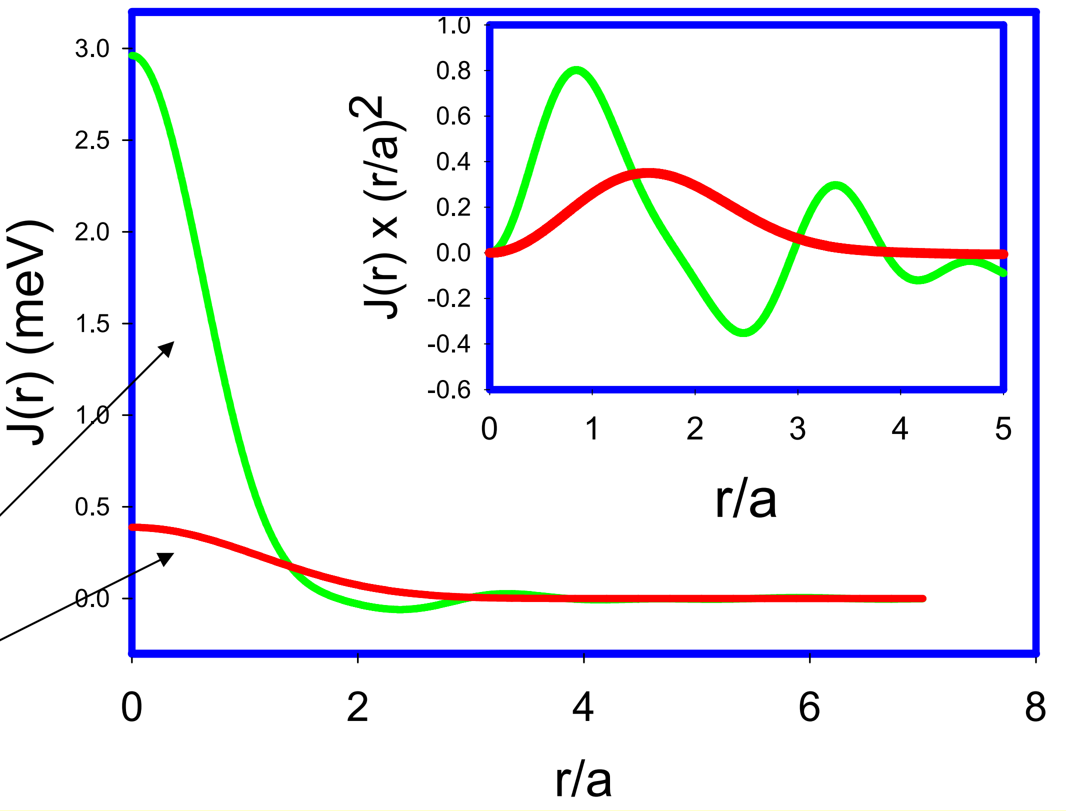
(disorder: random position of the Mn ions of the FCC lattice)

- Two-band model, m*=0.5
- Six band **k·p** model, GaAs

TWO BAND MODEL. ζ=0 **m*=0.5**

$p=4.4\times10^{20} cm^{-3}$
$J_{pd}=0.06$ eV nm^3

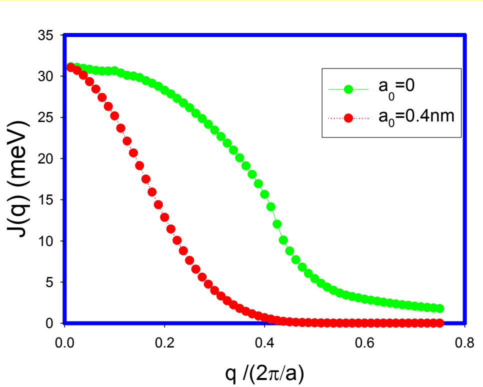


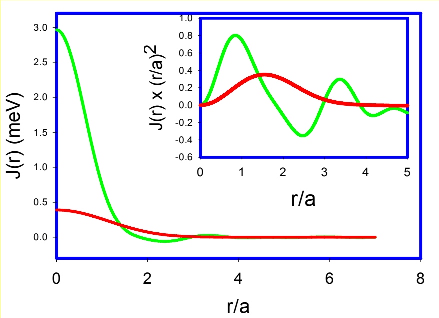


The same T_c^{vca}, but the effect of the fluctuations are very different.

TWO BAND MODEL. $\zeta=0$ $m^*=0.5$

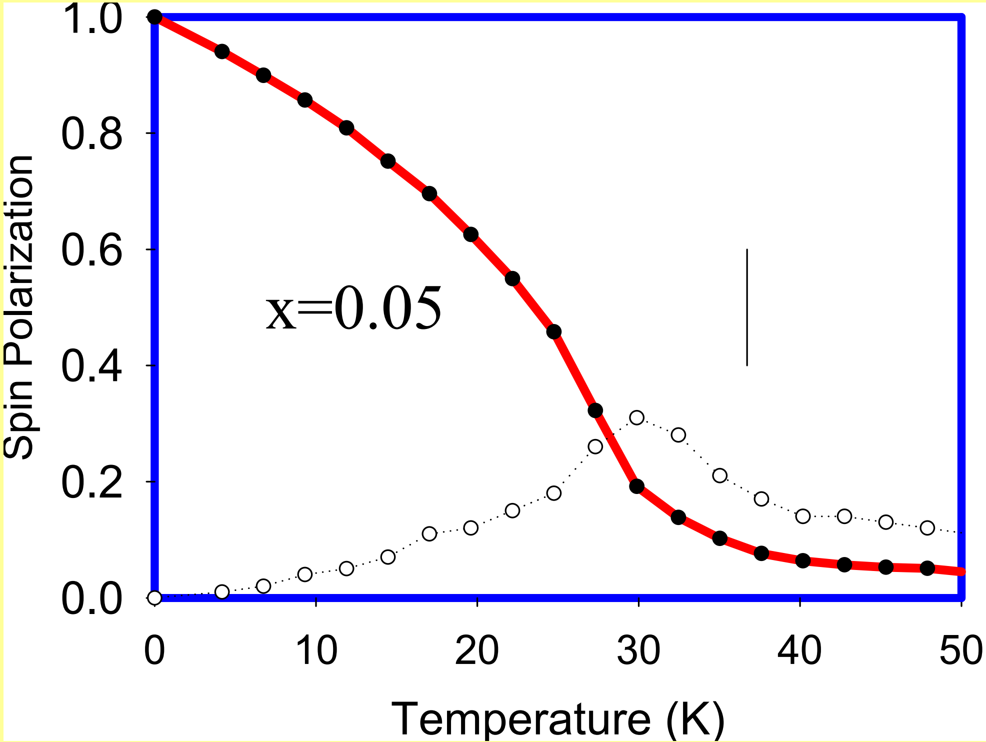
$p=4.4\times10^{20}cm^{-3}$
$J_{pd}=0.06$ eV nm^3





Monte Carlo (1350 Mn and 150 neighbors)

$a_0=0$
$a_0=0.16$nm
$T_c=0$

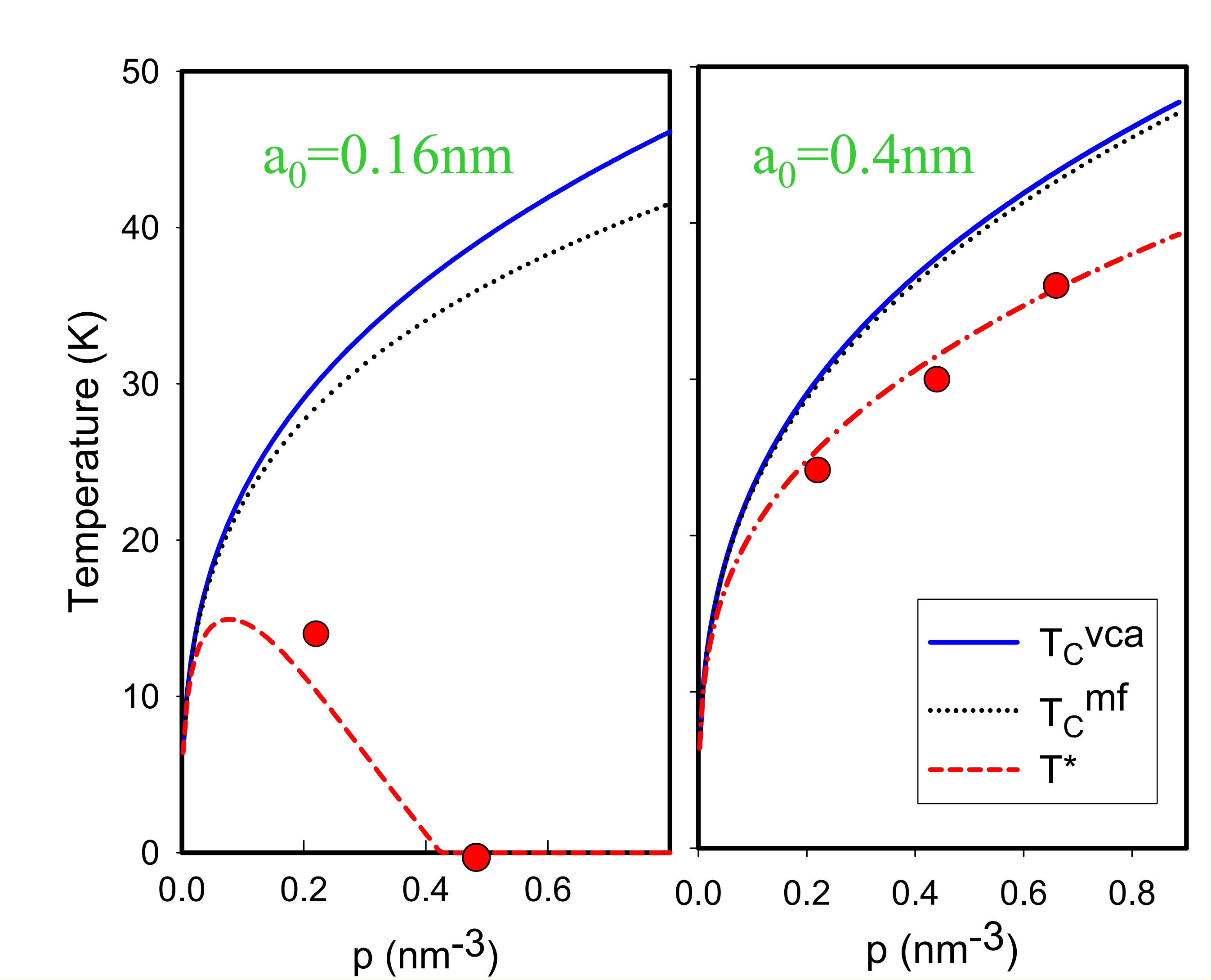


$a_0=0.4$nm
$T_c^{MF}=37K$
$T_c=30K$

TWO BAND MODEL m*=0.5

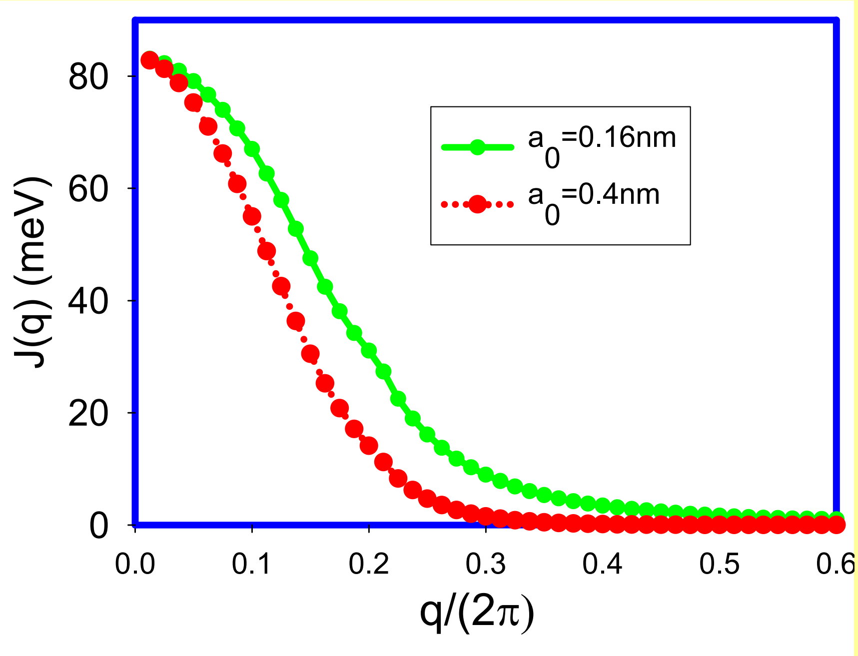
$x=0.05,\ J_{pd}=0.60\,\mathrm{eVnm}^3$

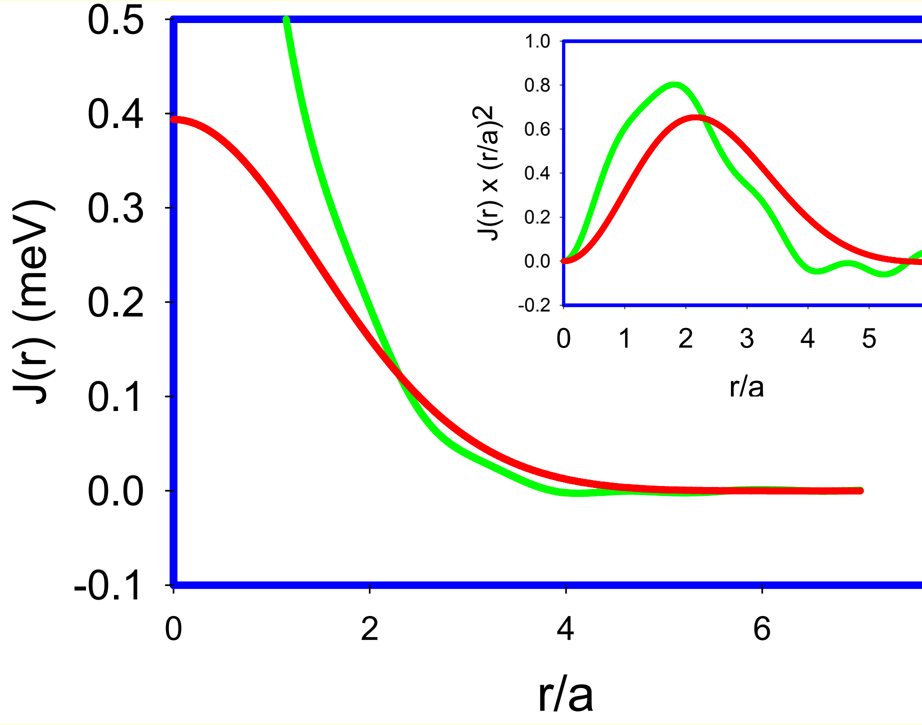
$$J(\vec{r}) = \frac{J_{pd}}{(2\pi a_0)^{3/2}} e^{-r^2/2a_0^2}$$

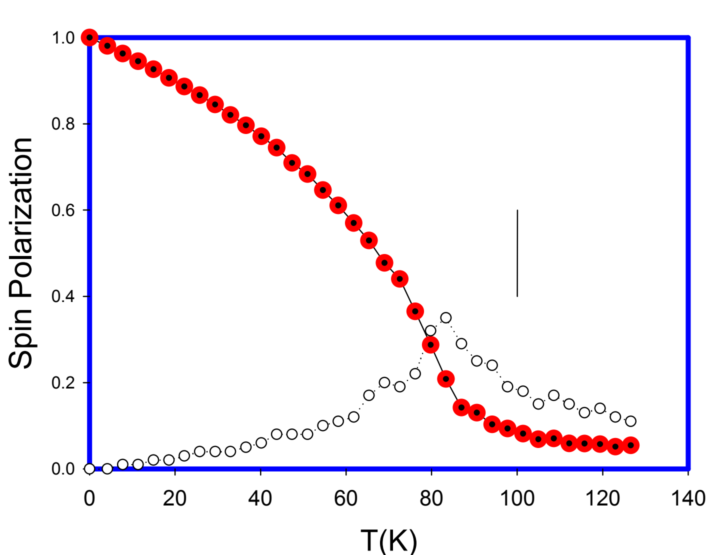


SIX K·P LUTTINGER MODEL GaAs

$p=4.4 \times 10^{20} cm^{-3}$
$J=0.06$ eV nm^3





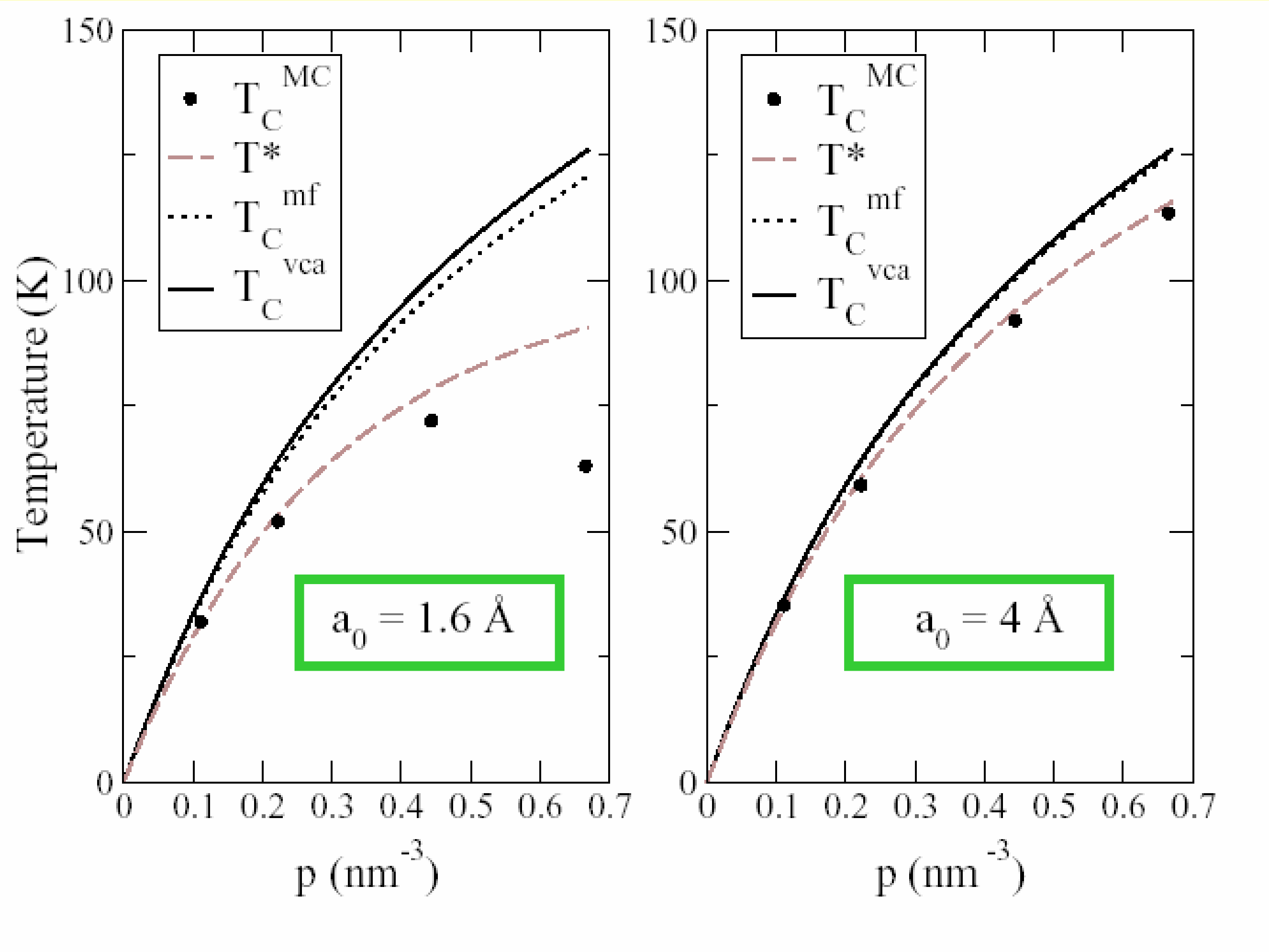


$a_0=0.16$nm, $T_c=83.4$K
$x=0.05$

SIX K·P LUTTINGER MODEL GaAs

p=4.4x10^{20}cm^{-3}
J=0.06 eV nm^3
x=0.05

$$J(\vec{r}) = \frac{J_{pd}}{(2\pi a_0)^{3/2}} e^{-r^2/2a_0^2}$$



Effect of quantum fluctuations and disorder on T=0 GS m=1 and ζ≠0.

Low energy magnetic excitations.

$$E = E_{KE}(\zeta) + \sum J_{I,J}(\zeta)\, \vec{S}_I \cdot \vec{S}_J$$

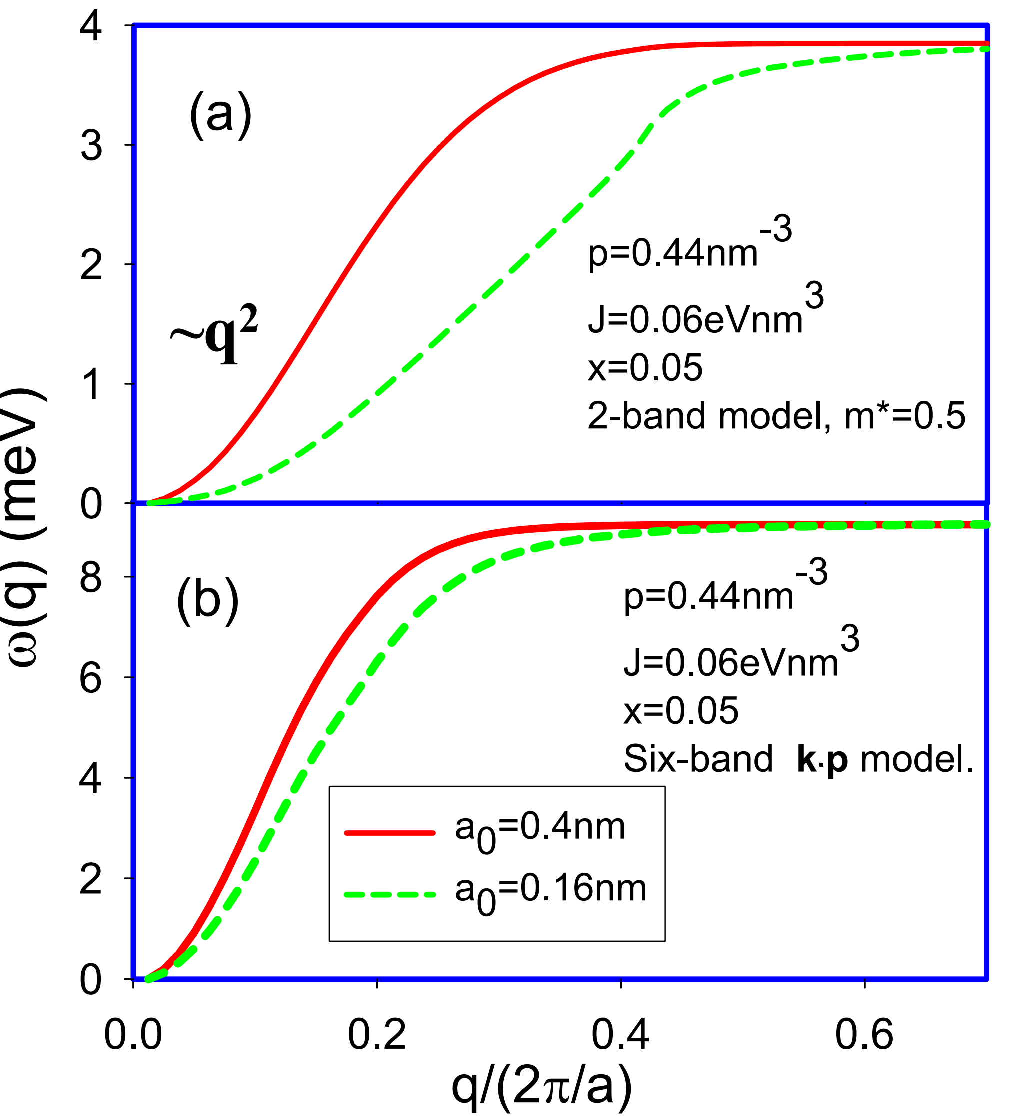
Spin Waves in VCA (all sites equivalents).

$$\Sigma_{\mathrm{Mn}} \rightarrow x\, \Sigma_{\mathrm{lattice}}$$

j runs over all lattice positions

$$\omega(q) = xS \sum_j J_{i,j}(1 - e^{-i\vec{q}\vec{R}_j}) = xSJ_{pd}^2 \left(\frac{a^3}{4} \right)^3 \left(\chi_\perp(0,\zeta) - \chi_\perp(q,\zeta) e^{-q^2 a_0^2} \right)$$

Spin Waves in VCA (all sites equivalents).



$$\omega(q)=\rho_s\, q^2/(2\pi/a)^2$$

	2-band	k·p
a_0=1.6Å	18meV	242meV
a_0=4Å	76meV	370meV

In agreement with Konig et al (00).

Effect of quantum fluctuations and DISORDER on GS ζ≠0

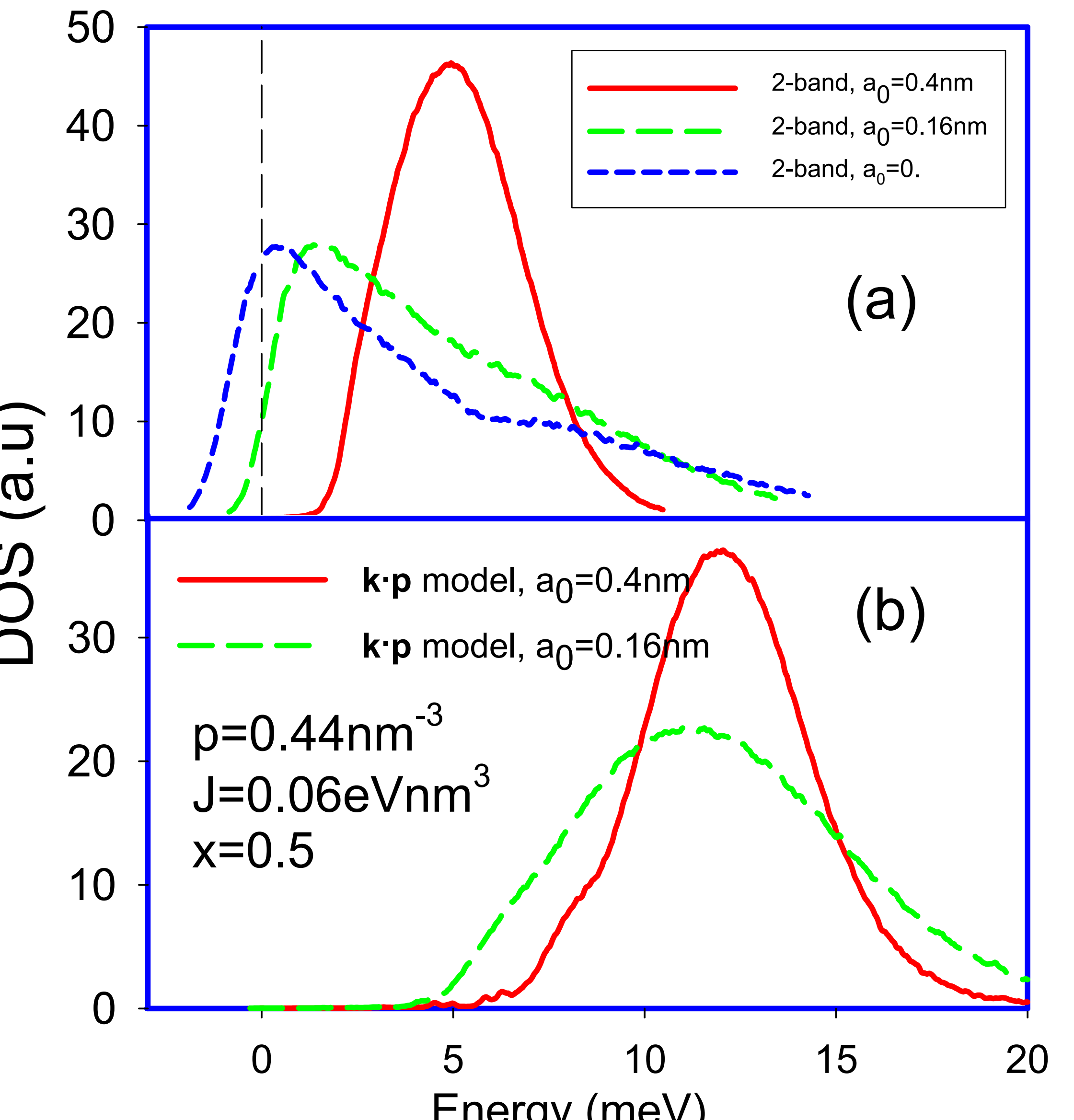
$$H = E(\zeta) + \sum J_{I,J}(\zeta)\, \vec{S}_I \cdot \vec{S}_J$$

Equation of motion method:

$$-i\hbar \frac{\partial S_I^-}{\partial t} = \left[H, S_I^-\right] = -\sum_J J_{I,J}\left(S_I^z S_J^- - S_J^z S_I^-\right)$$

Near T=0, S^z=S and the equation may be linearized. Numerically we solve systems with more than 500 Mn, with interaction up to 6a. (150 neighbors per Mn) and p.b.c. Since the system is disordered, we plot the collective spin excitation DOS. We average over several disorder realizations.

Disorder and quantum fluctuations (T=0).



In agreement with MC results!!!

Similar to Schliemann and MacDonald (perturbation theory, 2band) (2002) but different shape….

Up temperatures

T~5meV, $\Delta m(T) \sim T^{3/2}$

CONCLUSIONS

- We have developed a Heisenberg model for describing the magnetic properties of Diluted Magnetic Semiconductors. (GaMnAs). Large systems and using realistic band structures.
- Using this model we have study the effect of disorder, and thermal and quantum fluctuations on the properties of the DMS.
- It is important the use of an appropriated **k·p** model for describing the ferromagnetic phase. Two band model gives spurious non collinear ground states.

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$$H = H_0 + \Delta V$$

$$H = H^{\vec{k}\cdot\vec{p}}_{holes} + \underbrace{\sum_{I,i} \vec{S}_I \cdot \vec{s}_i \, J(\vec{R}_I - \vec{r}_i)}_{\Delta V}$$

- Mn have S=5/2.
- Mn are diluted and do not interact directly.
- Strong -AF- coupling between Mn spins and hole spins.

Note that i runs over all lattice sites,
And I runs just over the Mn locations

$$J(\vec{r}) = \frac{J_{pd}}{(2\pi a_0)^{3/2}} e^{-r^2/2a_0^2}$$

$$< n\vec{k} \,|\, \Delta V \,|\, n'\vec{k}' >= \frac{V J_{pd}}{N^2} \sum_I \alpha^{J,m_J}_{n,\vec{k}} \alpha^{J',m'_J}_{n',\vec{k}'} \; \vec{s}_{Jm_J,J'm'_J} \cdot \vec{S}_I \; e^{-i(\vec{k}'-\vec{k})\vec{R}_I} \; e^{-|\vec{k}-\vec{k}'|^2 \frac{a_0^2}{2}} (1-\delta_{\vec{k},\vec{k}'}$$

$$\varphi_{n,\vec{k}}(\vec{r},\zeta) = e^{i\vec{k}\vec{r}} \sum_{J,m_J} \alpha^{J,m_J}_{n,\vec{k}} u_{J,m_J}(\vec{r})$$

$$\varepsilon_{n,\vec{k}}(\zeta)$$

- $\vec{s}_{Jm_J,J'm'_J}$ *matrix element of the spin operator in the local angular momentum basis.*
- $\vec{S}_I$, $\vec{R}_I$ *Positions and orientations of the Mn spins.*
- a_0 *Cutoff in the reciprocal space. (range of th exchange interaction.)*

$$E = E_{KE} + \sum_{I,J} J_{I,J}(R_{I,J})\,\vec{S}_I \cdot \vec{S}_J$$

1. **Justification of the model.**

Effect of quantum fluctuations and disorder on the T=0 Ground State. $m=1, \zeta \neq 0$.

Study of the low energy magnetic excitations.

- Two-band model, $m^*=0.5$
- Six band **k·p** model, GaAs