RKKY Interaction in a monolayer MoS_2

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Outline

Intro.

- RKKY Interaction
- Applications

Formalism

- Green's function method
- Effect of Spin-Orbit coupling

RKKY MoS_2

- MoS_2 Effective Hamiltonian
- RKKY Int. in single layer MoS_2

Conclusion

- Results

Introduction

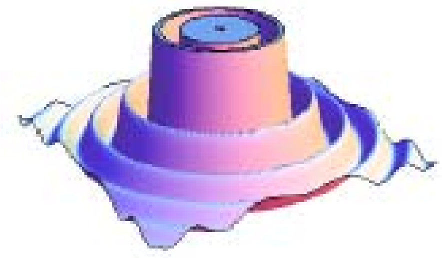
RKKY Interaction

Applications

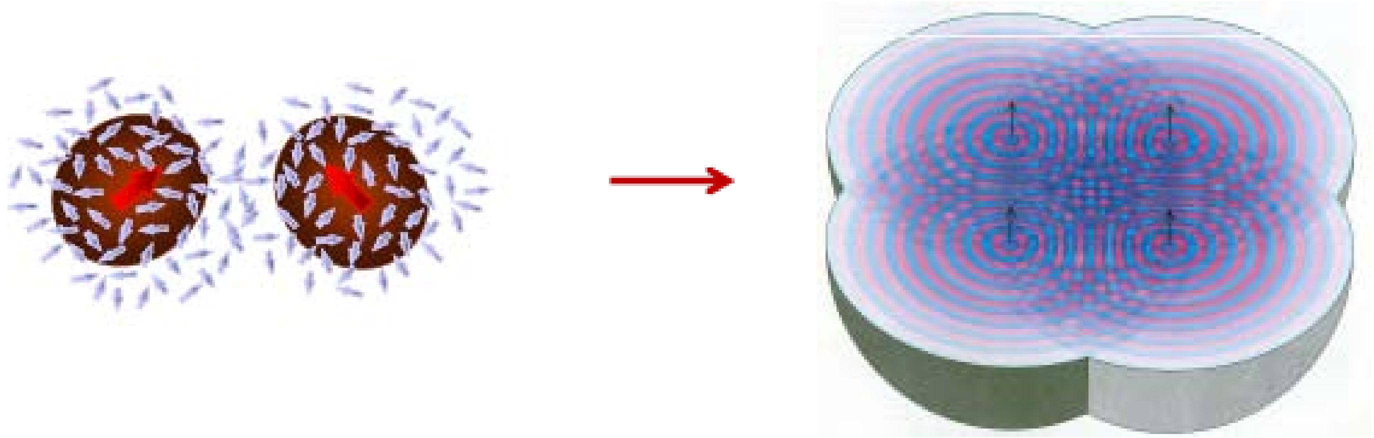
Magnetic impurities Interact via host electrons

- Electron spin oscillation around

Magnetic impurity



- Ordering of impurities:



RKKY Interaction (History)

- Interaction between nuclei spins (broadening of nuclear spin resonance line RKKY dominant over dipolar interaction)
- Rudermann and Kittel Phys. Rev. **96**,99
- Spontaneous nuclear spin polarization
- Interaction between localized electronic spins in metals (Ferro and anti ferromagnetism in metals)
- Kasuya Prog. of Theor. Phys. 16,45
- Interaction between magnetic Ad-atoms

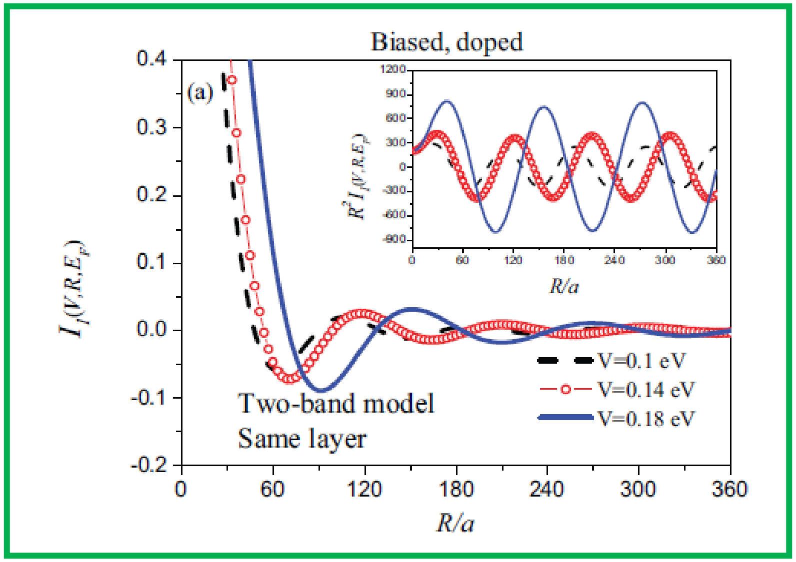
RKKY Interaction (Application)

- **Spintronic:**
- Increasing spin relaxation time to 200 μs
- Different types of spin Interaction
- Tuning spin transport properties

- **Ad-atom properties:**
- Magnetically doped materials
- Lattice defects

Important points in RKKY

- Interaction model
- Rate of decay
- Oscillation period
- Tunable parameters



- F.P., Sherafati, Asgari, Satpathy, Phys. Rev. B, 87, 165429

Formalism

Green's function method

Effect of spin-orbit interaction

RKKY Interaction

- Indirect Exchange interaction between two magnetic impurities via host conduction electrons

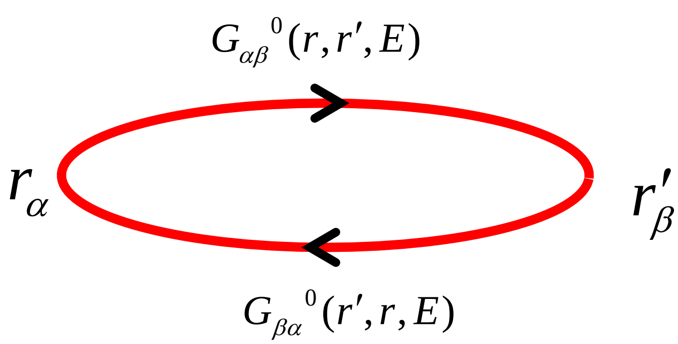
(Ruderman, Kittel, Kasuya, Yosida)

$$H = \lambda \sum_i S_1 . s_i + \lambda \sum_j S_2 . s_j$$

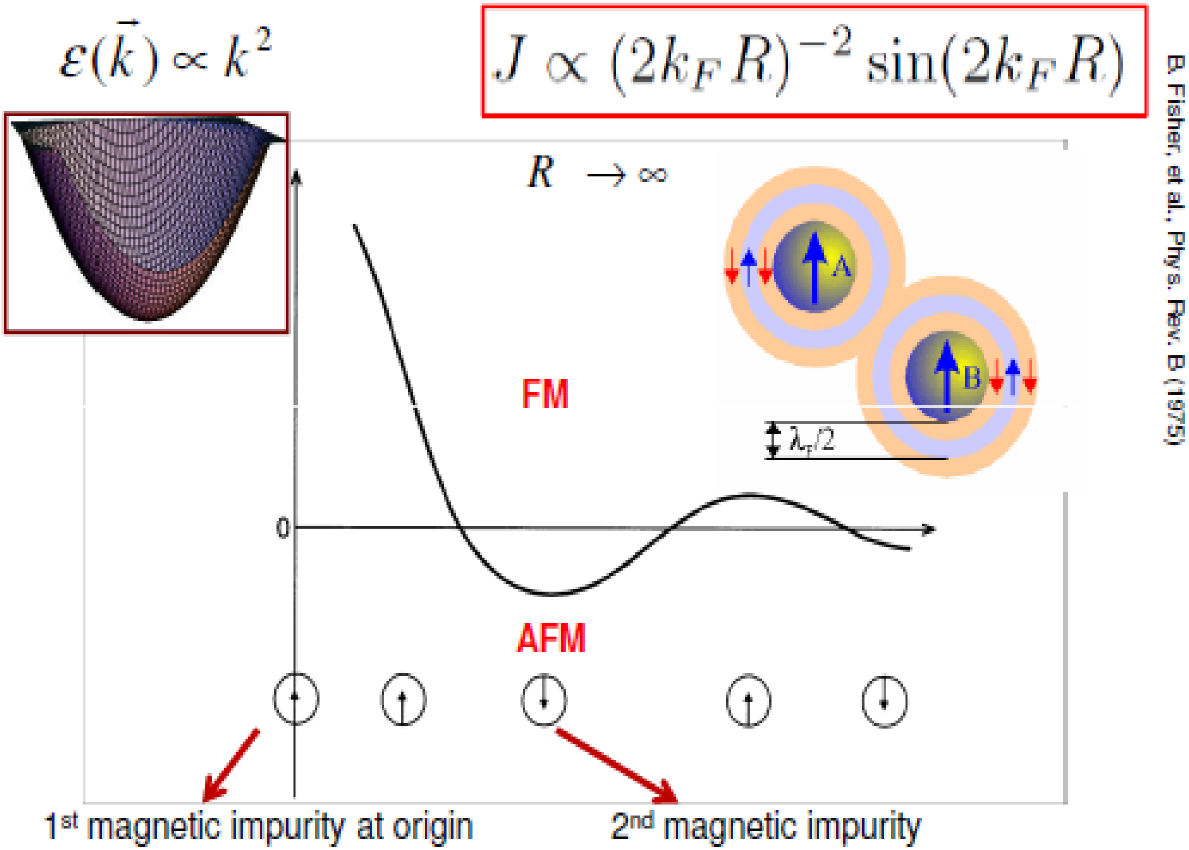
$$\hat{H}^{RKKY} = J \; S_1 . S_2$$

$$J(R) = \frac{\lambda^2 \hbar^2}{4} \chi(0, R)$$

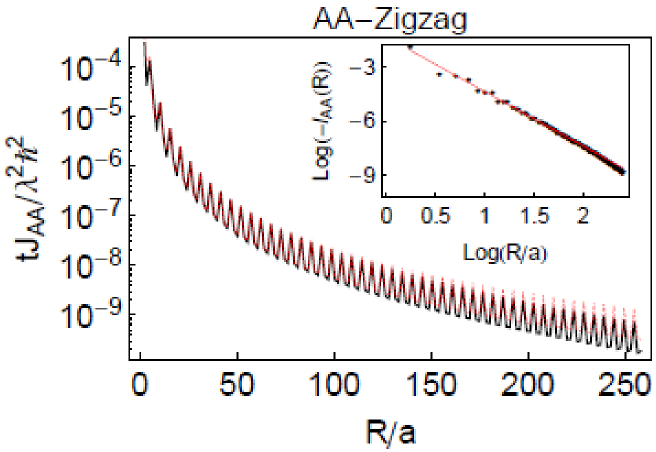
$$\chi(r, r') = -\frac{2}{\pi} \int_{-\infty}^{E_F} dE \, \mathrm{Im}[G^0(r, r', E) G^0(r', r, E)]$$

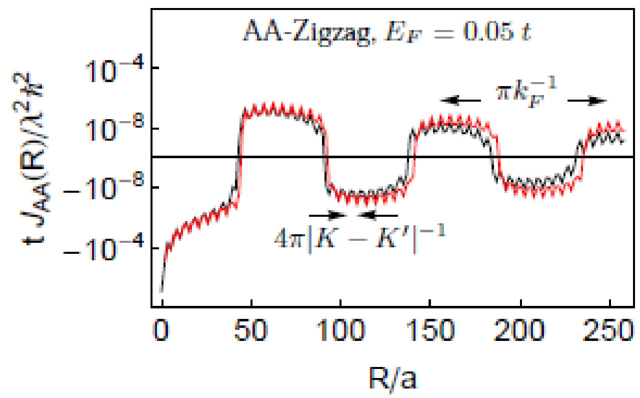


RKKY in 2DEG


$\varepsilon(\vec{k}) \propto k^2$
$J \propto (2k_F R)^{-2} \sin(2k_F R)$
B. Fisher, et al., Phys. Rev. B (1975)
$R \rightarrow \infty$
A
B
$\lambda_F/2$
FM
0
AFM
1st magnetic impurity at origin
2nd magnetic impurity

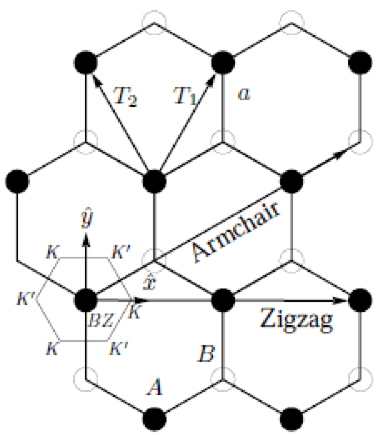
RKKY in Graphene





$$J_{AA} = C\frac{1+Cos((K-K').R)}{(R/a)^3}$$

$$J_{AA} = C\frac{1+Cos((K-K').R)}{(R/a)^2}Sin(2k_F R)$$



Sherafati et. al. PRB, **84**, 125416

Sherafati et. al. PRB, **83**, 165425

RKKY Interaction (spin system)

$$H_{RKKY} = -\lambda^2 \sum_{ij} I_{1i} \chi_{ij}(R_1, R_2) I_{2j}$$

$$i, j = x, y, z$$

$$\chi_{ij}(R_1, R_2) = \mathrm{Im}[\int_{-\infty}^{\varepsilon_F} d\varepsilon Tr[\hat{\sigma}_i G^0(R_1, R_2, \varepsilon)\hat{\sigma}_j G^0(R_2, R_1, \varepsilon)]$$

$$G = \begin{pmatrix} g^{\uparrow\uparrow} & g^{\uparrow\downarrow} \\ g^{\downarrow\uparrow} & g^{\downarrow\downarrow} \end{pmatrix}$$

RKKY in spin polarized systems

- Different Models:
- Spin degenerate:

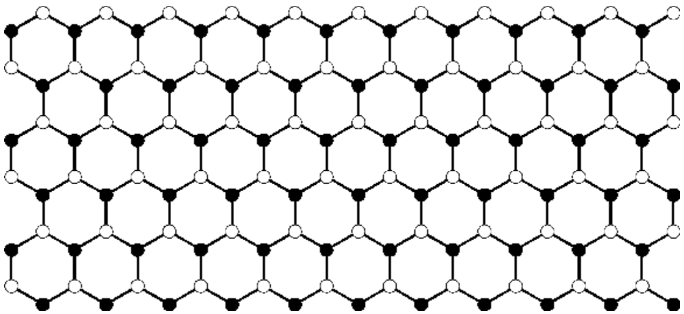
$$G = \begin{pmatrix} g & 0 \\ 0 & g \end{pmatrix} \Rightarrow \hat{H} = J I_1 . I_2$$

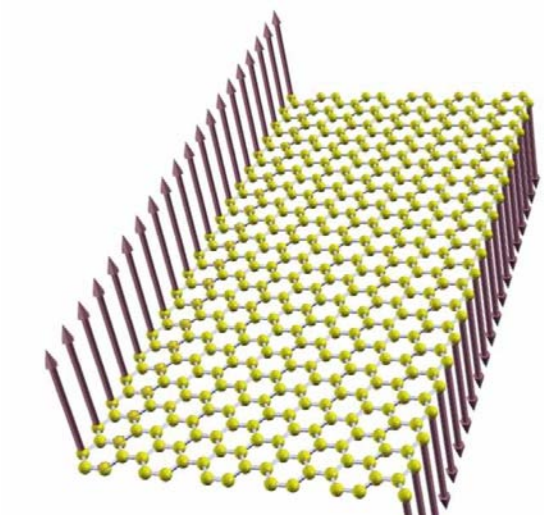
- Spin-polarized OR +spin-orbit :

$$G = \begin{pmatrix} g^{\uparrow} & 0 \\ 0 & g^{\downarrow} \end{pmatrix} \Rightarrow \hat{H} = J_x (I_{1x} I_{2x} + I_{1y} I_{2y}) + J_z I_{1z} I_{2z}$$

RKKY in spin polarized Graphene

$$H^{\alpha\beta}{}_{RKKY} = \frac{\lambda^2}{\pi}[J_x^{\alpha\beta}(S_{1x}S_{2x} + S_{1y}S_{2y}) + J_z^{\alpha\beta}(S_{1z}S_{2z}]$$





F.P., Asgari, Abedinpour, Zareyan, PRB, **87**, 125402

RKKY in 2DEG+Rashba S.O.

$$\hat{H} = \frac{-\hbar^2}{2m^*}\nabla^2 + \alpha(-i\hbar\nabla \times \hat{z}).\sigma \Rightarrow G = \begin{pmatrix} g_0 & -ig_1 \\ ig_1 & g_0 \end{pmatrix}$$

$$\Rightarrow \hat{H}^{RKKY} = F_1(|R_{12}|)\{\cos(2k_F R_{12})S_1.S_2 + \sin(2k_F R_{12})(S_1 \times S_2)_y$$
$$+[1-\cos(2k_F R_{12})]S_1^y S_2^y\}$$

- Heisenberg + Ising + D.M.
- Rotating S_2 by $\theta_{12} = 2k_F R_{12}$ around y $\Rightarrow$
- Heisenberg model

PRB **69** , 121303 (R) (2004)

RKKY in Topological Insulator

$$\hat{H} = \hbar v_F (k_x\sigma_x + k_y\sigma_y) \Rightarrow G = \begin{pmatrix} g_0 & g_1 - ig_2 \\ g_1 + ig_2 & g_0 \end{pmatrix}$$

$$\Rightarrow \hat{H}^{RKKY} = F_1(|R_{12}|)S_1.S_2 + F_2(|R_{12}|)(S_1 \times S_2)_y + F_3(|R_{12}|)S_1^y S_2^y$$

- Heisenberg + Ising + DM

PRL **106** , 097201(2011)

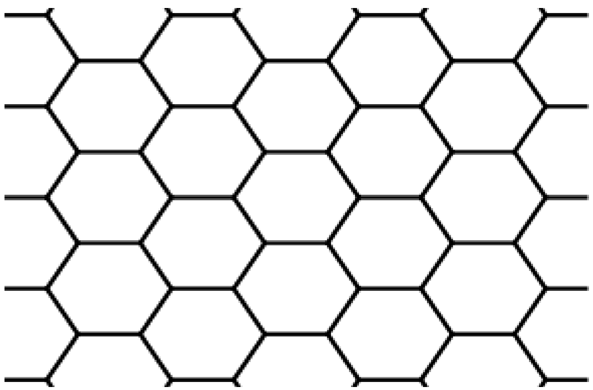
RKKY Interaction in MoS_2

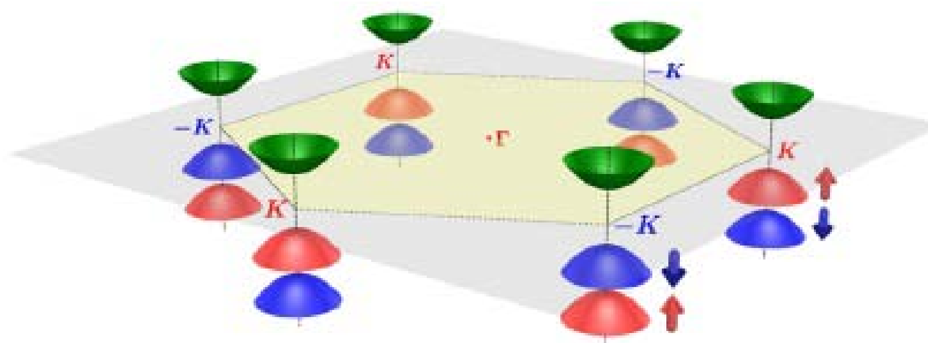
MoS_2 Effective Hamiltonian

RKKY Int. in single layer MoS_2

Single Layer MoS_2: Interesting Properties of Honeycomb Lattice

- Valley Degeneracy
- Massive Dirac Fermions
- Special strong spin-orbit coupling
- Effect of time reversal symmetry



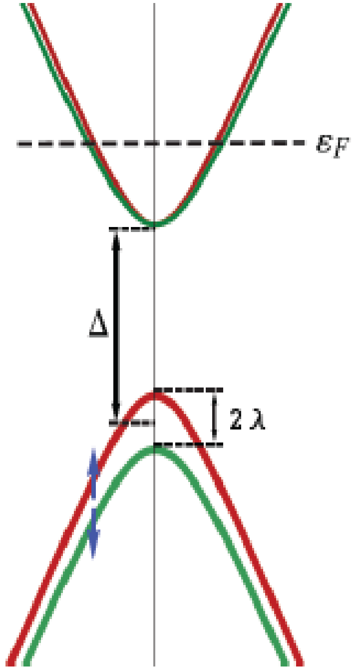


MoS_2 Hamiltonian Model

$$\hat{H} = at(\tau k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) + \frac{\Delta}{2}\hat{\sigma}_z - \lambda\tau\frac{\hat{\sigma}_z - 1}{2}\hat{s}_z$$

τ , σ , s $\rightarrow$ pauli matrices in valley , band , spin spaces

	a	Δ	t	2λ	Ω_1	Ω_2
MoS_2	3.193	1.66	1.10	0.15	9.88	8.26
WS_2	3.197	1.79	1.37	0.43	15.51	9.57
$MoSe_2$	3.313	1.47	0.94	0.18	10.23	7.96
WSe_2	3.310	1.60	1.19	0.46	16.81	9.39



RKKY Interaction in MoS_2

- Re-writing Hamiltonian:

$$\hat{\mathcal{H}}_0^\tau = \begin{pmatrix} \Delta/2 & at\tau k e^{-i\tau\theta'} & 0 & 0 \\ at\tau k e^{i\tau\theta'} & -\Delta/2+\lambda\tau & 0 & 0 \\ 0 & 0 & \Delta/2 & at\tau k e^{-i\tau\theta'} \\ 0 & 0 & at\tau k e^{i\tau\theta'} & -\Delta/2-\lambda\tau \end{pmatrix}$$

$$H_{RKKY}^{\alpha\beta} = -\lambda^2 \sum_{ij} I_{1i}\chi_{ij}(R_1, R_2) I_{2j}$$

$$\chi_{ij}(R_1, R_2) = \mathrm{Im}[\int_{-\infty}^{\varepsilon_F} d\varepsilon Tr[\hat{\sigma}_i G(R_1, R_2, \varepsilon)\hat{\sigma}_j G(R_2, R_1, \varepsilon)]$$

RKKY Interaction in MoS_2

$$G(R,0,\varepsilon)=\begin{pmatrix} e^{iK.R}g_- + e^{iK'.R}g_+ & 0 \\ 0 & e^{iK.R}g_- + e^{iK'.R}g_+ \end{pmatrix}$$

$$G(0,R,\varepsilon)=\begin{pmatrix} e^{-iK.R}g_- + e^{-iK'.R}g_+ & 0 \\ 0 & e^{-iK.R}g_- + e^{-iK'.R}g_+ \end{pmatrix}$$

$$\hat{H}^{RKKY} = J_H S_1.S_2 + J_I S_1{}^z S_2{}^z + J_{DM}(S_1 \times S_2)_z$$

- Where

$$J_H \square\ 4g_+g_- + 2(g_+{}^2 + g_-{}^2)\cos((K-K').R)$$

$$J_I \square\ 2(g_+ - g_-)^2(1-\cos((K-K').R))$$

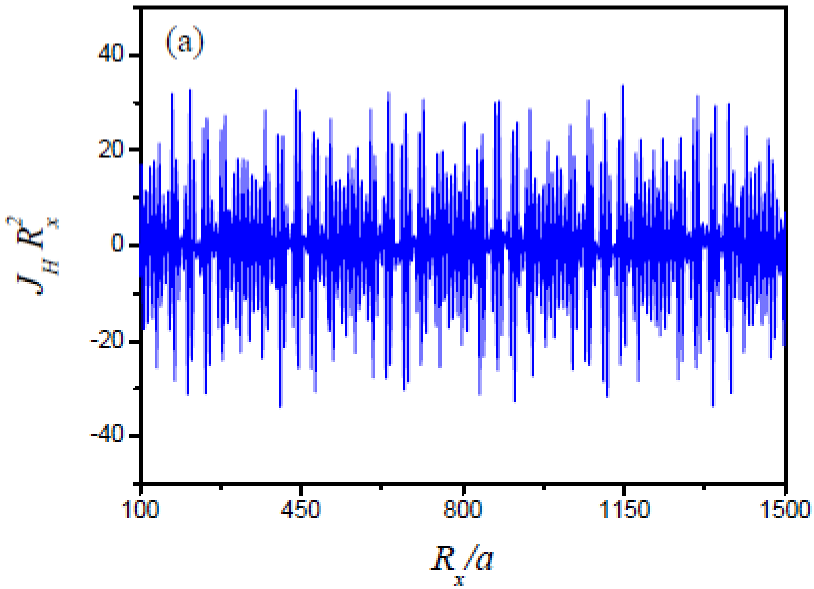
$$J_{DM} \square\ -2(g_+{}^2 - g_-{}^2)\sin((K-K').R)$$

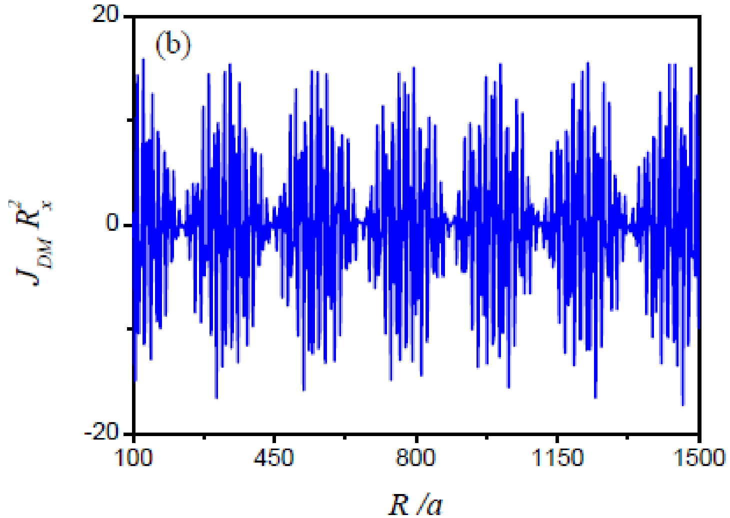
- existence of DM term without spin twisting

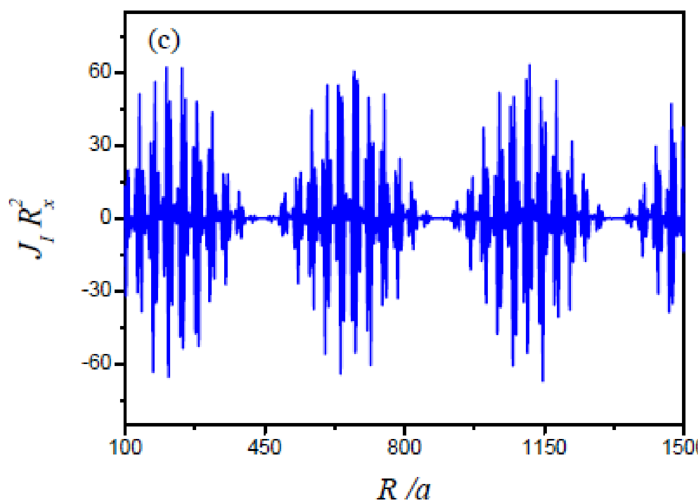
Numerical Results

Results

- Long Range Behaviour:

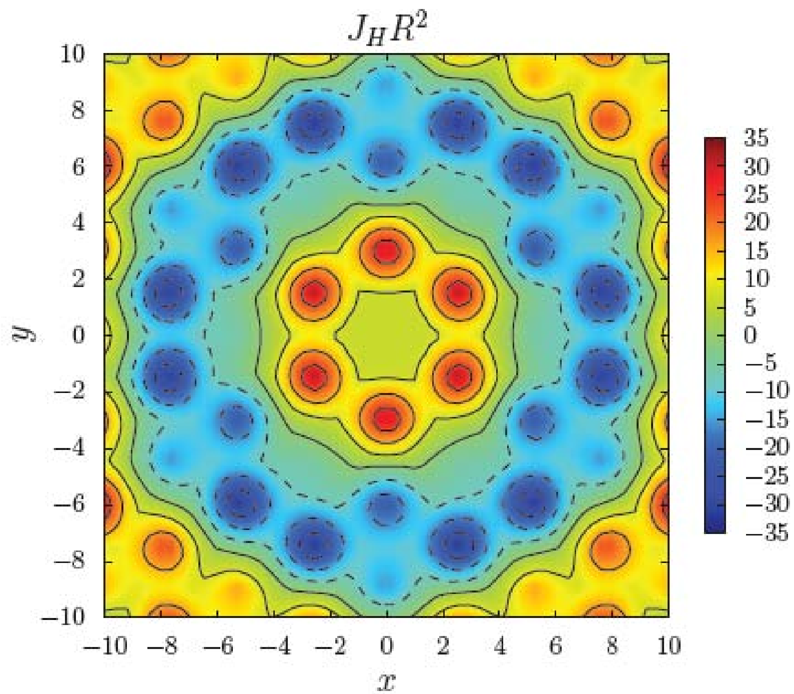


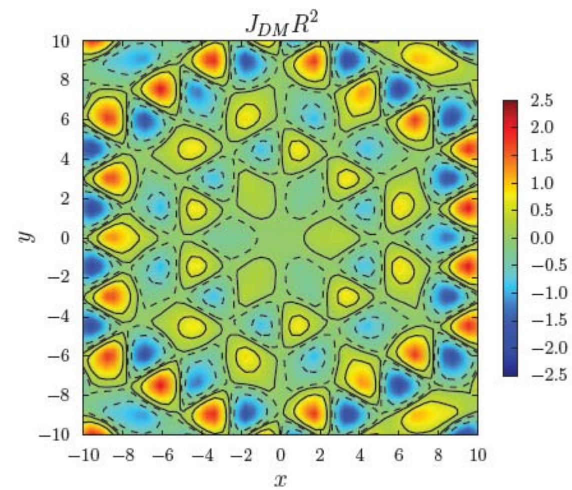


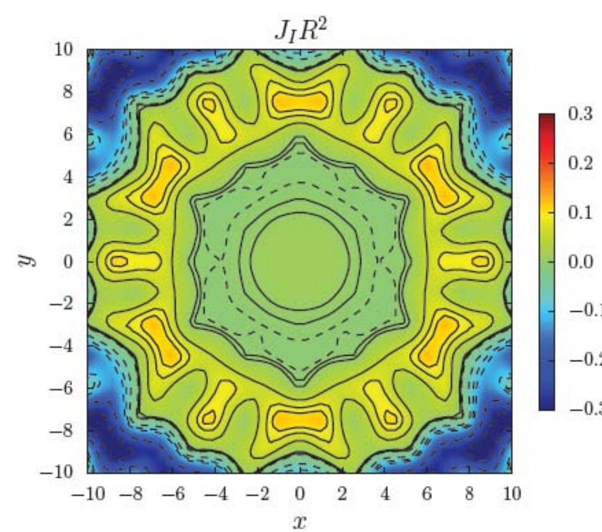


Results

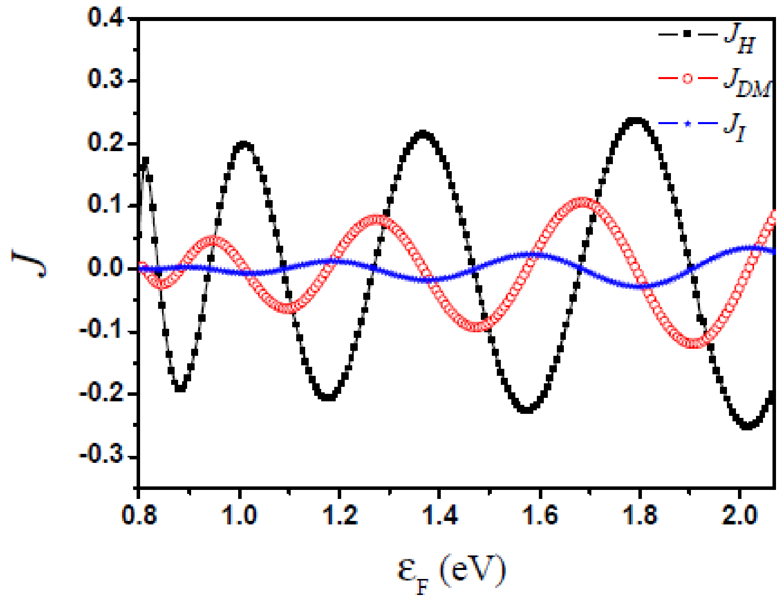
- Short Range counter plot:



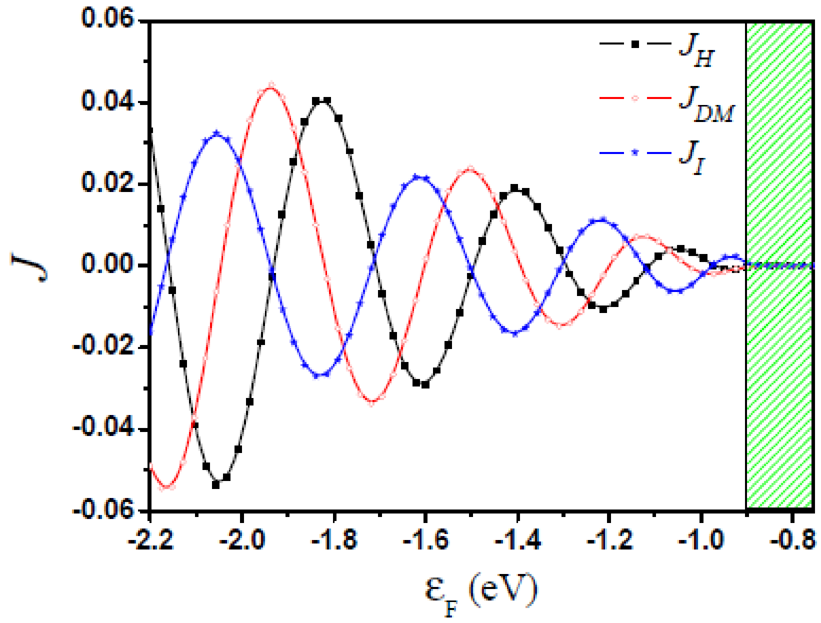




Results



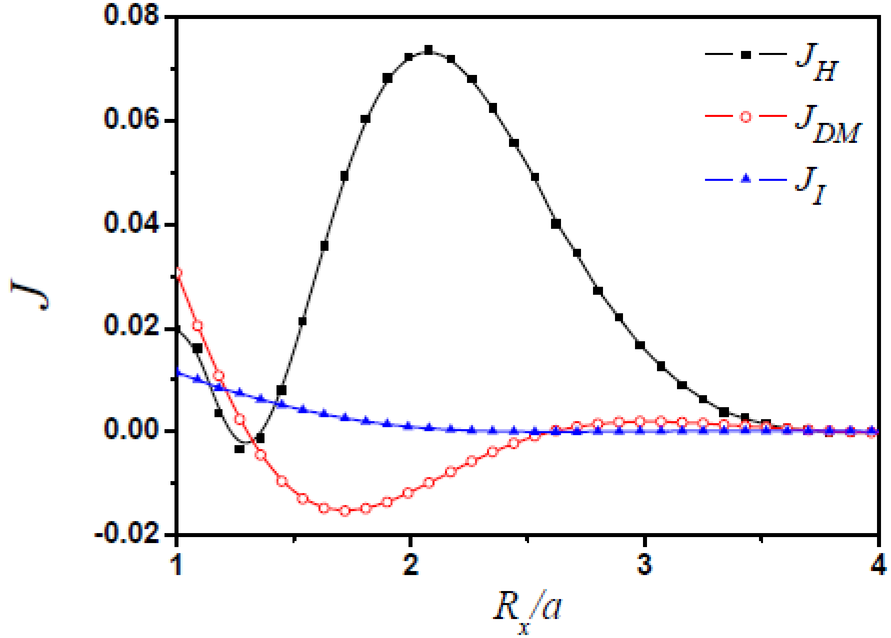
0.4
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
J
0.8
1.0
1.2
1.4
1.6
1.8
2.0
ε_F (eV)
J_H
J_DM
J_I



0.06
0.04
0.02
0.00
-0.02
-0.04
-0.06
J
-2.2
-2.0
-1.8
-1.6
-1.4
-1.2
-1.0
-0.8
ε_F (eV)
J_H
J_DM
J_I

Results

- Short Range interaction (BR)



Results

- Rotation of magnet moments:

$$
\begin{aligned}
-(J_H + J_I)\cos\theta_2 \sin\theta_1 + \sin\theta_2 \cos\theta_1 (J_H \cos\phi + J_{DM}\sin\phi) &= 0 \\
-(J_H + J_I)\cos\theta_1 \sin\theta_2 + \sin\theta_1 \cos\theta_2 (J_H \cos\phi + J_{DM}\sin\phi) &= 0 \\
\sin\theta_1 \sin\theta_2 (-J_H \sin\phi + J_{DM}\cos\phi) &= 0
\end{aligned}
$$

$$\theta_1, \theta_2 = 0, \pi$$

$$\theta_1 = \theta_2 = \frac{\pi}{2}$$

$$\phi = \tan^{-1}\left(J_{DM} / J_H \right)$$

$$
\begin{aligned}
D_1 &= -sign(J_H)\sqrt{J_H^2 + J_{DM}^2} \\
D_2 &= J_{DM}^2 - J_I(2J_H + J_I)
\end{aligned}
$$

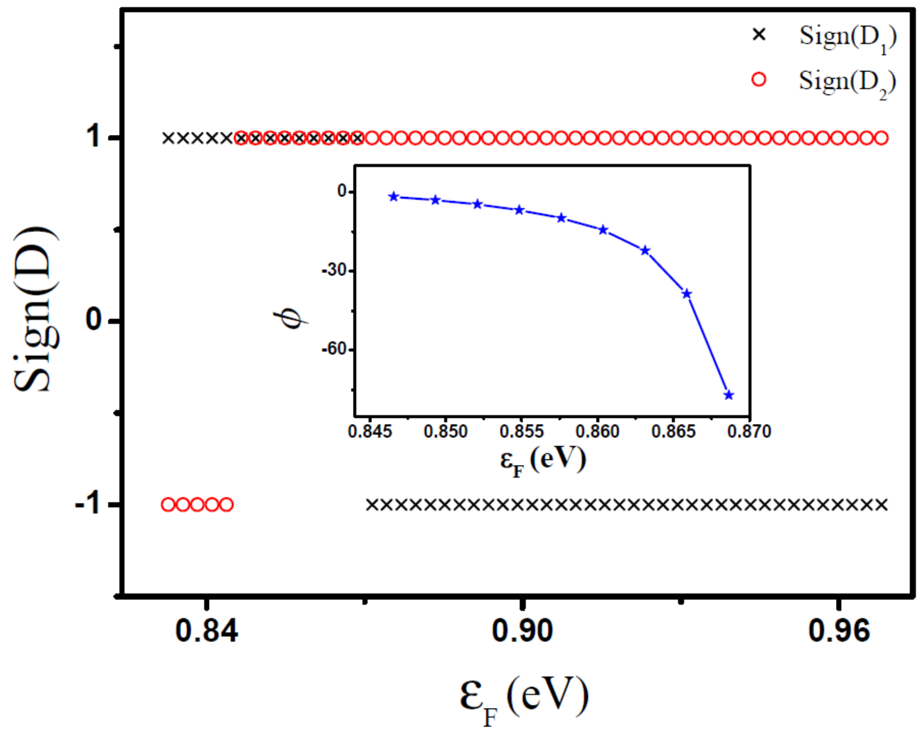
$D_1 > 0, D_2 > 0$ $\quad \theta = \frac{\pi}{2}$ is a min.

$D_1 < 0, D_2 > 0$ $\quad \theta = \frac{\pi}{2}$ is a max.

otherwise $\quad \theta = \frac{\pi}{2}$ is a saddle point.

Results

- Angle of rotation:



F.P., Rostami, Asgari, Phys. Rev. B , 87, 125401


Thanks For your Attention