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#### Introduction to RKKY interaction

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#### Summary

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Introduction

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Introduction

#### History

Introduction

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History





Figure: Malvin Ruderman and Charles Kittel

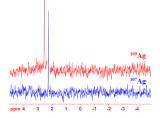


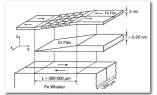
Figure: Resonance peaks of  $^{109}A_g$  and  $^{107}A_a$ 

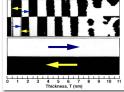
# The problem of the large nuclear spin resonance in pure silver

- 1953 N.Bloembergen and J.Rowland measured the effects of multi-polar momentum on the shift of nuclear resonance rays for tin, lead and thallium of nuclear isospin  $I > \frac{1}{2}$
- measurement of the magnetic order in a layer or alloys
- Silver has isospin  $I = \frac{1}{2} \longrightarrow$  no multi-polar momentum  $\longrightarrow$  no shift expected
- Measurements show a small shift but broad resonance peak (5x larger than expected)
- Happens also for other atomic layers of isospin  $I = \frac{1}{2}$  ⇒ General behavior due to the layer's structure!

Source: http://chem.ch.huji.ac.il/nmr/
techniques/1d/row5/ag.html

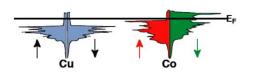
#### Strange Observations in Quantum Wells and Transistors





J. Unguris et al., Phys. Rev. Lett. **67**, 140 (1991)

Figure: Current transmission in a layer of increasing thickness



100 - 1 Tod. 2 K O RT K

Figure: Resistivity for two materials of increasing thickness

Figure: Spin reflectivity for two metals

Source: https://www.fz-juelich.de/SharedDocs/Downloads/PGI/PGI-6/DE/Lec\_2009-01-06red\_pdf.pdf?\_\_blob=publicationFile

#### History

Introduction

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Figure: Tadao Kasuva and Kei Yosida

#### The problem of the large nuclear spin resonance in pure silver

- Introduce a particle which carries the spin information from one atom to an other one.
- ⇒ Applicant's profile :
  - charged particle
  - propagates "free" in metals
  - fermion of spin  $\frac{1}{2}$
  - interacts with the nucleus through hyperfine interaction
- ⇒ electron meets the job requirements!
- => Extension of the model to condensed matter

0000 History

#### History

#### How to make an electron connect two atoms far away one from an other?



Basics of Quantum Mechanics

Figure: Free electron / Delocalized electron

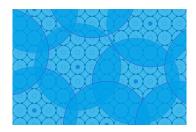


Figure: Doped semi-conductor's electrons / d-shell electrons

See also: M. A. RUDERMAN AND C. KITTEL, "Indirect Exchange Coupling of Nuclear Magnetic Moments by Conduction Electrons", PHYSICAL REVIEW VOLUME 96, NUMBER 1 OCTOBER 1, 1954

See also: N. Bloembergen and T. J. Rowland, "ON THE NUCLEAR MAGNETIC RES-ONANCE IN METALS AND ALLOYS "Acta Metallurgica 1, 731 (1953).

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Basics of Quantum Mechanics

Introduction

#### Exchange Operator

Consider two particles in a system and the exchange operator  $\hat{P}$ :

$$\hat{P} \ket{\Psi(\mathbf{r_1}, \mathbf{r_2})} = \ket{\Psi(\mathbf{r_2}, \mathbf{r_1})}$$

 $\implies$  Is  $\hat{P}$  an Observable compatible with  $\hat{H}$ ?

$$\begin{split} \langle \Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)|\left[\hat{P},\hat{H}\right]|\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle &= \langle \Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)|\left(\hat{P}\hat{H}-\hat{H}\hat{P}\right)|\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle \\ &= \langle \Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)|\left.\hat{P}\hat{H}|\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle - \langle \Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)|\left.\hat{H}\hat{P}\right|\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle \right. \\ &= \mathcal{E}\left\langle \Psi(\boldsymbol{r}_2,\boldsymbol{r}_1)|\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle - \mathcal{E}\left\langle \Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)|\Psi(\boldsymbol{r}_2,\boldsymbol{r}_1)\rangle \right. \\ &= 0 \end{split}$$

 $\implies$  A complete set of functions that are simultaneous eigenstates of  $\hat{H}$  and  $\hat{P}$  exists.

 $\Longrightarrow$  It is possible to measure the values of  $\hat{H}$  and  $\hat{P}$  simultaneously!

Eigenvalues of  $\hat{P}$  are +1 and -1

 $\Longrightarrow$  A quantum system evolves in a state which preserves the initial symmetry of the system.

Introduction

Spin Operator

### Construction of the spin on the same way than an angular momentum.

$$\hat{S} = egin{pmatrix} \hat{S}_{\mathsf{x}} \ \hat{S}_{\mathsf{y}} \ \hat{S}_{\mathsf{z}} \end{pmatrix}$$

Commutation properties:

$$[\hat{S}_i, \hat{S}_j] = i \ \varepsilon_{i,j,k} \ \hat{S}_k$$

Eigenvalues of spin Observables:

$$\hat{S^2} \ket{s,m_s} = s(s+1)\ket{s,m_s}$$

$$\hat{S}_{z}|s,m_{s}\rangle=m_{s}|s,m_{s}\rangle$$

The spin operator is not an observable compatible with the Hamiltonian!

Heisenberg relation:

$$-i\frac{\mathrm{d}\hat{A}}{\mathrm{d}t} = [\hat{H}, \hat{A}]$$

 $\implies [\hat{H}, \hat{A}] = 0$  only for  $\hat{A} = \hat{S}_z$  and  $\hat{A} = \hat{S}^2 \implies$  Only  $\hat{S}_z$  and  $\hat{S}^2$  are conserved!

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### Spin Operator for two particles

Construction of the total spin operator.

Basics of Quantum Mechanics

$$\hat{S} = \hat{S_1} + \hat{S_2}$$

Commutation properties:

$$[\hat{S}_1, \hat{S}_2] = 0$$
  $[\hat{S}_{1z}, \hat{S}_1] = 0$   $[\hat{S}_{1x,v}, \hat{S}_1] \neq 0$ 

Let's build a ensemble of Observables which commutes with themselves and with the Hamiltonian:

$$\left\{\hat{S^2}, \hat{S^2_1}, \hat{S^2_2}, \hat{S^2_{1,z}}, \hat{S^2_{2,z}}\right\}$$

Let's assume a continuum of accessible states:

$$\underbrace{\hat{S}^2}_{\text{Total spin}} = \underbrace{\hat{S}^2_1}_{\text{On site 1}} + \underbrace{\hat{S}^2_2}_{\text{On site 2}} + 2 \underbrace{\hat{S}_1 \cdot \hat{S}_2}_{\text{Exchange}}$$

Eigenvalues of the square spin operators for electrons are  $\frac{3}{4}$  for  $\hat{S^2_\tau}$  and  $\hat{S^2_\tau}$ 

Eigenvalues of  $\hat{S}^2$  are 0 if s=0 and 2 if s=1.

If 
$$s = 0 \longrightarrow \hat{S}_1 \cdot \hat{S}_2$$
 has eigenvalue  $-\frac{3}{4}$   
If  $s = 1 \longrightarrow \hat{S}_1 \cdot \hat{S}_2$  has eigenvalue  $\frac{1}{4}$ 

### Perturbation theory

Introduction

Consider a Hamiltonian in two parts : main unperturbed  $\hat{H}_0$  and perturbed by a field  $F(t) = F(t)\Theta(t - t_0)$  and an operator  $\hat{B}$ :

$$\hat{H} = \hat{H_0} + F(t)\Theta(t - t_0)\hat{B}$$

 $\Theta(t-t_0)$  is the causality!

Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \ket{\psi(t)} = \hat{H} \ket{\psi(t)}$$

Not convenient to solve → assume time evolution is also an operator (interaction picture)

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi\rangle$$

Time operator's properties:

$$\hat{U}(t,t_0) = e^{-i\hbar\hat{H}_0(t-t_0)}\hat{U}_I(t,t_0)$$

⇒ Solve Schrödinger equation!

$$i\hbar \frac{\partial}{\partial t} \hat{U}_I(t,t_0) = F(t)\Theta(t-t_0)\hat{B}(t-t_0)\hat{U}_I(t,t_0)$$

 $\implies$  Everything happens as if the unperturbed Hamiltonian  $\hat{H}_0$  was taken as the new origin of energy!

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#### Perturbation theory

Introduction

Perturbation theory

Goal: We want to know the value of an Observable  $\hat{A}$ !

General expression of the time operator ( $1^{st}$  order):

$$U_l(t,t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t F(s)B(s-t_0)\mathrm{d}s$$

Average value of an observable in time:

$$\langle A \rangle (t) = \langle \Psi(t) | A | \Psi(t) \rangle$$

And at thermal equilibrium:

$$\langle A \rangle_{eq} = \langle \Psi | A | \Psi \rangle$$

Then, the response of the system with respect to thermal equilibrium :

$$\left\langle A\right\rangle (t)-\left\langle A\right\rangle =-rac{i}{\hbar}\int_{0}^{t-t_{0}}\Theta( au)\left\langle \left[A( au),B
ight]
ight
angle F(t- au)\mathrm{d} au=\int_{0}^{t-t_{0}}\chi_{AB}( au)F(t- au)\mathrm{d} au$$

Thus:

$$\chi_{AB}(\tau) = -\frac{i}{\hbar}\Theta(\tau)\langle [A(\tau), B]\rangle$$

#### Perturbation theory

Introduction

$$\chi_{AB}(\tau) = -\frac{i}{\hbar}\Theta(\tau)\langle [A(\tau), B]\rangle$$

Let's explain the commutator:

Expression of the operator in a orthogonal basis:

$$A = \sum_{lpha,eta} A_{lpha,eta} a_{lpha}^{\dagger} a_{eta} \qquad B = \sum_{\gamma,\delta} B_{\gamma,\delta} a_{\gamma}^{\dagger} a_{\delta}$$

with the time evolution properties:

$$a_{\alpha}(t) = e^{-\frac{i}{\hbar}\varepsilon_{\alpha}t}a_{\alpha}$$
  $a_{\alpha}^{\dagger}(t) = e^{\frac{i}{\hbar}\varepsilon_{\alpha}t}$ 

and commutations properties:

$$\left[a_{lpha}^{\dagger}a_{eta},a_{\gamma}^{\dagger}a_{\delta}
ight]=\delta_{eta,\gamma}a_{lpha}^{\dagger}a_{\delta}-\delta_{lpha,\delta}a_{\gamma}^{\dagger}a_{eta}$$

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Introduction

# $\chi_{AB}(\tau) = -\frac{i}{\hbar}\Theta(\tau)\langle [A(\tau), B]\rangle$

Insert in green equation:

$$\chi_{AB}(\tau) = -\frac{i}{\hbar}\Theta(\tau)\sum_{\alpha,\beta,}A_{\alpha,\beta}B_{\beta,\alpha}\,e^{\frac{i}{\hbar}(\varepsilon_{\alpha}-\varepsilon_{\beta})\tau}\bigg(f(\varepsilon_{\alpha})-f(\varepsilon_{\beta})\bigg)$$

with the occupation rates given by the Fermi-Dirac distribution:

$$f(\varepsilon) = \frac{1}{e^{\frac{\varepsilon - \mu N}{k_B T}} + 1}$$

Finally, make the Fourier transform in time:

$$\chi_{AB}(q,\omega) = \left(rac{(2\pi)^d}{V}
ight)^2 \sum_{lpha,eta} A_{lpha,eta} B_{eta,lpha} rac{f(arepsilon_lpha) - f(arepsilon_eta)}{\hbar\omega + (arepsilon_lpha - arepsilon_eta) + i\hbar\eta}$$

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Introduction

Perturbation theory

$$\chi_{AB}(q,\omega) = \left(rac{(2\pi)^d}{V}
ight)^2 \sum_{lpha,eta,} A_{lpha,eta} B_{eta,lpha} \, rac{f(arepsilon_lpha) - f(arepsilon_eta)}{\hbar\omega + (arepsilon_lpha - arepsilon_eta) + i\hbar\eta}$$

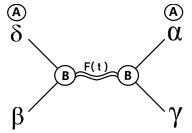


Figure: Feynman's diagram representation of the response function in linear response theory

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#### Atomic Model

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# $H = \sum_{i} \frac{p_{i}^{2}}{2\mu_{i}} + V_{p-e}(r_{i}) + \sum_{i} \underbrace{V_{X}(r_{i})}_{Exchange} + \underbrace{V_{e-e}(r_{i})}_{Resonant \ interaction} + \underbrace{V_{corr}(r_{i})}_{Correlations}$ Between sites

See also: D. R. Hartree, PROC. CAMB. PHILOS. SOC, 24, 89, 111 ET 426 (1928)

#### Hydrogen Atom

Introduction
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Hydrogen atom

- Solve Schrödinger equation
- Wave functions fills the whole space
- Extend the model to many electrons



Figure: Hydrogen atom

# Hydrogen wave functions

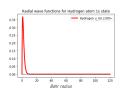
$$n = 1$$

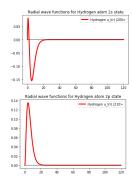
Introduction

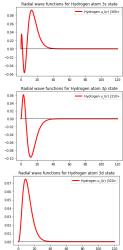
Hydrogen atom

$$n=2$$









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#### Extension to Helium atom

$$H = \sum_{i} \frac{p_{i}^{2}}{2\mu_{i}} + V_{p-e}(r_{i}) + \sum_{i} \underbrace{V_{X}(r_{i})}_{Exchange} + \underbrace{V_{e-e}(r_{i})}_{Resonant \ interaction} + \underbrace{V_{corr}(r_{i})}_{Correlations}$$
Between sites

See also: D. R. Hartree, PROC. CAMB. PHILOS. SOC, 24, 89, 111 ET 426 (1928)

#### Helium Atom

Introduction

Helium atom and other atoms

- Solve Schrödinger equation with Hartree potential
- Wave functions modified
- Extend the model to many atoms without a lot of particles

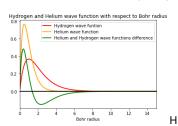


Figure: Helium atom

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#### Extension to other atoms

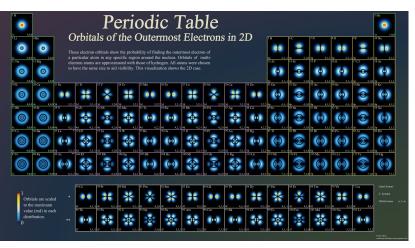


Figure: Periodic Table of Elements for Physicists

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#### Extension to Di-Hydrogen

$$H = \underbrace{\sum_{i} \frac{p_{i}^{2}}{2\mu_{i}} + V_{p-e}(r_{i})}_{On \ site} + \underbrace{\sum_{i} \underbrace{V_{X}(r_{i})}_{Exchange} + \underbrace{V_{e-e}(r_{i})}_{Resonant \ interaction} + \underbrace{V_{corr}(r_{i})}_{Correlations}$$

See also: D. R. Hartree, PROC. CAMB. PHILOS. SOC, 24, 89, 111 ET 426 (1928)

#### Di-Hydrogen

- Solve Schrödinger equation with all terms
- Wave functions impossible to get analytically
- Extend the model to many atoms without a lot of particles

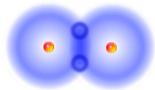


Figure: Di-Hydrogen electron cloud

#### Extension to Crystals

$$H = \sum_{i} \frac{p_{i}^{2}}{2\mu_{i}} + V_{p-e}(r_{i}) + \sum_{i} \underbrace{V_{X}(r_{i})}_{Exchange} + \underbrace{V_{e-e}(r_{i})}_{Resonant \ interaction} + \underbrace{V_{corr}(r_{i})}_{Correlations}$$

$$= \underbrace{V_{Corr}(r_{i})}_{Between \ sites}$$

See also: D. R. Hartree, PROC. CAMB. PHILOS. SOC, 24, 89, 111 ET 426 (1928)

#### Crystals

Introduction

Crystals

- $10^{23}$  atoms
- Impossible to solve Schrödinger equation analytically

#### Simplify the Hamiltonian

- Assume to know the exact electronic wave function of each electron
- Reduce the problem to many identical

⇒ Identical particles ⇔ Problem solved ⇒ Introduce the Spin!

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Heisenberg Model

#### Exchange energy between two particles

Consider a system of two particles in the following total state:

$$|\Psi_{1,2}\rangle = \underbrace{|\psi(\mathbf{r_1}, \mathbf{r_2})\rangle}_{\text{spatial part}} \underbrace{|\chi(s_1, s_2)\rangle}_{\text{spin part}}$$

Suppose identical particles

For fermions, the total state has to be anti symmetric.

If the spin part is symmetric:

If the spin part is anti-symmetric:

- ⇒ spatial part is anti-symmetric
- $\implies$  the spins are parallels

⇒ spatial part is anti-symmetric

⇒ the spins are anti-parallels

Singlet spin state

Triplet spin state 
$$\Rightarrow S = 1, m_S = \{-1, 0, 1\}$$

$$\Longrightarrow S = 0, m_s = 0$$

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If the spin part is symmetric:

- ⇒ spatial part is anti-symmetric
- ⇒ the spins are parallels

$$\ket{\Psi_{1,2}}_{\mathit{Sym}} = rac{\ket{\psi_1(\mathbf{r_1})}\ket{\psi_2(\mathbf{r_2})} - \ket{\psi_2(\mathbf{r_1})}\ket{\psi_1(\mathbf{r_2})}}{\sqrt{2}}\ket{\chi_{\mathit{Sym}}}$$

Energy of this state:

Introduction Two particles system

$$\begin{split} E_{\mathcal{S}\chi} &= \left\langle \Psi_{1,2} \right|_{\mathcal{S}ym} \hat{H} \left| \Psi_{1,2} \right\rangle_{\mathcal{S}ym} \\ &= \int \psi_{\mathcal{S}ym} (\mathbf{r_1}, \mathbf{r_2})^* \hat{H} \psi_{\mathcal{S}ym} (\mathbf{r_1}, \mathbf{r_2}) \mathrm{d} \mathbf{r_1} \mathbf{r_2} \times \left\langle \chi_{\mathcal{S}ym} \right| \hat{H} \left| \chi_{\mathcal{S}ym} \right\rangle \\ &= \frac{3}{4} E_{\mathcal{S}} \end{split}$$

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If the spin part is symmetric:

- ⇒ spatial part is anti-symmetric
- ⇒ the spins are parallels

$$\left|\Psi_{1,2}\right\rangle_{\textit{Anti-Sym}} = \frac{\left|\psi_{1}(\textbf{r_{1}})\right\rangle\left|\psi_{2}(\textbf{r_{2}})\right\rangle + \left|\psi_{2}(\textbf{r_{1}})\right\rangle\left|\psi_{1}(\textbf{r_{2}})\right\rangle}{\sqrt{2}}\left|\chi_{\textit{anti-sym}}\right\rangle$$

Energy of this state:

Introduction Two particles system

$$\begin{split} E_{T\chi} &= \left\langle \Psi_{1,2} \right|_{\textit{Anti-Sym}} \hat{H} \left| \Psi_{1,2} \right\rangle_{\textit{Anti-Sym}} \\ &= \int \psi_{\textit{Anti-Sym}} (\textbf{r_1},\textbf{r_2})^* \hat{H} \psi_{\textit{Anti-Sym}} (\textbf{r_1},\textbf{r_2}) \mathrm{d}\textbf{r_1}\textbf{r_2} \times \left\langle \chi_{\textit{anti-sym}} \right| \hat{H} \left| \chi_{\textit{anti-sym}} \right\rangle \\ &= \frac{1}{4} E_T \end{split}$$

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#### The total wave function is given by

$$|\Psi_{tot}
angle = |\psi_{\mathcal{S}}
angle + |\psi_{\mathcal{T}}
angle$$

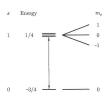


Figure: Energy levels of a two particle state

#### Total energy:

Introduction

$$\begin{split} E_{tot} &= \left\langle \Psi_{tot} \right| \hat{H} \left| \Psi_{tot} \right\rangle \\ &= \left\langle \psi_{S} \right| \hat{H} \left| \psi_{S} \right\rangle + \left\langle \psi_{T} \right| \hat{H} \left| \psi_{T} \right\rangle + \left\langle \psi_{S} \right| \hat{H} \left| \psi_{T} \right\rangle + \left\langle \psi_{T} \right| \hat{H} \left| \psi_{S} \right\rangle \\ &= \frac{3}{4} E_{S} + \frac{1}{4} E_{T} - (E_{S} - E_{T}) \left[ \left\langle \chi_{anti-sym} \right| \hat{S_{1}} \cdot \hat{S_{2}} \left| \chi_{sym} \right\rangle + \left\langle \chi_{sym} \right| \hat{S_{1}} \cdot \hat{S_{2}} \left| \chi_{anti-sym} \right\rangle \right] \\ &= \frac{3}{4} E_{S} + \frac{1}{4} E_{T} - 2(E_{S} - E_{T}) \left\langle \chi_{anti-sym} \right| \hat{S_{1}} \cdot \hat{S_{2}} \left| \chi_{sym} \right\rangle \end{split}$$

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The total wave function is given by

$$|\Psi_{tot}
angle = |\psi_{\mathcal{S}}
angle + |\psi_{\mathcal{T}}
angle$$

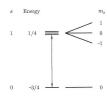


Figure: Energy levels of a two particle state

Therefore:

$$\hat{H} = E_{flat} - J\hat{S}_1 \cdot \hat{S}_2$$
  $\rightarrow$   $J > 0$   $\rightarrow$  anti-symmetric spatial part  $\rightarrow$  minimizes the Coulomb repulsion

With

Introduction

$$J = 2(E_{S} - E_{T}) = 2 \int \psi_{1}(\mathbf{r_{1}})\psi_{2}(\mathbf{r_{2}})\hat{H}\psi_{1}(\mathbf{r_{2}})\psi_{2}(\mathbf{r_{1}})\mathrm{d}\mathbf{r_{1}}\mathrm{d}\mathbf{r_{2}}$$

Extend to a lattice:

$$\hat{H} = \underbrace{E_{flat}}_{On \; site} - \sum_{i,j} \underbrace{J_{i,j} \hat{S}_i \cdot \hat{S}_j}_{Spin \; Exchange}$$

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Basics of Quantum Mechanics Atomic Model Heisenberg Model 000000 Heisenberg interaction Hamiltonian

#### Physical properties of Heisenberg model

Introduction

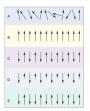


Figure: Different magnetism

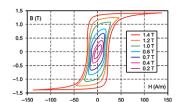


Figure: Ferromagnetic Hysteresis loop

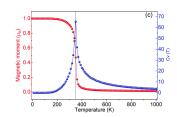


Figure: Curie temperature and specific heat of a ferromagnetic system

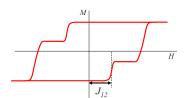


Figure: Ferromagnetic Hysteresis loop

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#### **RKKY Interaction**

**RKKY Interaction** 

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#### Extension of the Heisenberg Model

Note : for far away particles,  $J \rightarrow 0$ 

⇒ introduce a particle which will carry the interaction
→ delocalized electrons of the lattice : *d*-shells or free electrons

Note: Heisenberg model is an internal description of a system!

$$\hat{H}_{\mathit{int}} = -J \sum_{i} \hat{S}_{i} \cdot \hat{\sigma} \delta(\mathbf{r} - \mathbf{r_{i}}) \quad o \quad \hat{H}_{\mathit{int}} = g \mu_{\mathit{B}} \sum_{i} H_{\mathit{eff}} \cdot \hat{\sigma}$$

Each electron interacts with an effective magnetic field given by the internal contribution of each spin :

$$H_{eff} = -rac{J}{g\mu_B}\hat{S}_i\delta(\mathbf{r}-\mathbf{r_i})$$

This effective fields links the macroscopic magnetization and the microscopic spins :

$$M(\mathbf{r}) = \int \chi(\mathbf{r} - \mathbf{r}') H_{\text{eff}}(\mathbf{r}') d\mathbf{r}' = -\frac{J}{g\mu_B} \chi(\mathbf{r}) \hat{S}_i = -g\mu_B \sigma(\mathbf{r})$$

Where :  $\chi(\mathbf{r})$  is the response function of the electron  $\sigma(\mathbf{r})$  is the spin density of the system

RKKY Interaction

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Note : for far away particles,  $J \rightarrow 0$ 

 $\implies$  introduce a particle which will carry the interaction  $\rightarrow$  delocalized electrons of the lattice : d-shells or free electrons

Note: Heisenberg model is an internal description of a system!

$$\hat{H}_{int} = -J \sum_{i} \hat{S}_{i} \cdot \hat{\sigma} \delta(\mathbf{r} - \mathbf{r_{i}}) \quad \rightarrow \quad \hat{H}_{int} = g \mu_{B} \sum_{i} H_{eff} \cdot \hat{\sigma}$$

Each electron interacts with an effective magnetic field given by the internal contribution of each spin :

$$H_{ extstyle extstyle H_{ extstyle extstyle H_{ extstyle B}} \hat{S}_i \delta(\mathbf{r} - \mathbf{r_i})$$

$$\hat{H}_{\mathsf{RKKY}} = -rac{J^2}{(g\mu_{\mathsf{B}})^2} \sum_{i,j} \chi(\mathbf{r_{i,j}}) \hat{S}_i \cdot \hat{S}_j$$

Main goal now : what is  $\chi(\mathbf{r_{i,i}})$  ?

### RKKY response function

From second order of perturbation theory:

$$\chi(\mathbf{r},t) = \int \int \int \frac{f(\mathbf{k}) - f(\mathbf{k}')}{\hbar\omega + \varepsilon \mathbf{k} - \varepsilon \mathbf{k}' - i\eta} e^{i[(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r} - \omega t]} d\mathbf{k} d\mathbf{k}' d\omega$$

Fermi-Dirac distribution:

$$f(\mathbf{k}) = \frac{1}{1 + e^{\frac{\varepsilon_{\mathbf{k}} - \varepsilon_{F}}{k_{B}T}}}$$

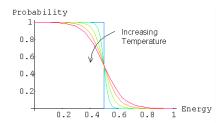


Figure: Fermi-Dirac distribution

Complicated integral → Approximation

Sommerfeld's expansion:

$$\int_0^\infty f(k)g(k)k\mathrm{d}k = \int_0^{k_F} g(k)k\mathrm{d}k + \frac{\pi^2}{24} \left(\frac{T}{T_F}\right)^2 k_F^3 \frac{\mathrm{d}g(k)}{\mathrm{d}k}\Big|_{k_F}$$

Valid for small temperatures and small ranges:

$$\frac{T}{T_F} > \frac{1}{2k_F r}$$

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## RKKY response function

#### What gives the integration in 2D?



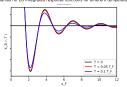


Figure: RKKY analytical response function

Comparison of 2D Integrated and Analytic response functions for T = 0.1Tf

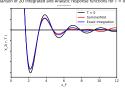


Figure: RKKY analytical and exact response functions

$$\chi_{2}(r,T) = -\frac{m}{2\pi\hbar^{2}}k_{F}^{2} \left[ J_{0}(k_{F}r)Y_{0}(k_{F}r) + J_{1}(k_{F}r)Y_{1}(k_{F}r) - \frac{\pi^{2}}{12} \left( \frac{T}{T_{F}} \right)^{2} k_{F}r \left( J_{1}(k_{F}r)Y_{0}(k_{F}r) + J_{0}(k_{F}r)Y_{1}(k_{F}r) \right) \right]$$

#### Important behaviors to note:

- lacksquare divergence at r=0 o Pauli principle.
- Long range vanishing → recovering the constraints of Heisenberg model.

#### New behavior : Oscillations !

- Favored positions of the atoms in the lattice
- Source of Giant Magneto-Resistance

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Introduction

#### RKKY measurements in materials

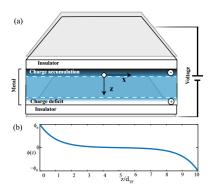


Figure: Experimental setup

Source: Alejandro O. Leon et Al., "Manipulation of the RKKY exchange by voltages", PHYSICAL REVIEW B 100, 014403 (2019), DOI: 10.1103/PhysRevB.100.014403

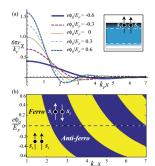


Figure: RKKY susceptibility between two particles at the interface with an insulator

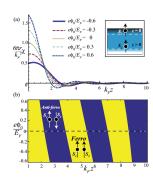


Figure: RKKY susceptibility between two particles at two different interfaces with two insulators

Source: Alejandro O. Leon et Al., "Manipulation of the RKKY exchange by voltages", PHYSICAL REVIEW B 100, 014403 (2019), DOI: 10.1103/PhysRevB.100.014403

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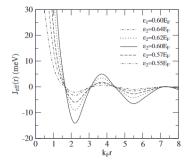


Figure: RKKY magnetic interaction between two localized spins at several different carrier energy levels e2 with the fixed energy level  $\varepsilon_1 = 0.6 E_F$ , the fixed hybridization strength V = 8.0 meV nm, and the fixed density of the semiconductor  $n = 4.0 \times 10^{11} cm^{-2}$ 

Source: Yao-Rui Wu, Dan Wang, and Pin Lyu, "Ruderman-Kittel-Kasuya-Yosida interaction between diluted magnetic semiconductor quantum dots embedded in semiconductor", JOURNAL OF APPLIED PHYSICS 112, 063905 (2012), http://dx.doi. org/10.1063/1.4752401

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# Giant Magneto Resistance

Introduction

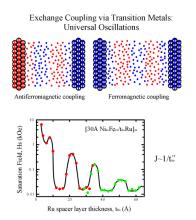


Figure: Giant Magneto-resistance in a 30A thick NiFeRu layer

Source: "Magnetoresistance - Giant MagnetoResistance (GMR) and Tunnelling MagnetoResistance (TMR)", http://www.almaden.ibm.com/st/

Summary

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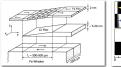
Basics of Quantum Mechanics

Atomic Model

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#### Summary

Introduction





Observations of different conductivity in thin metallic layers depending on the spin of the electrons

Figure: Current transmission in a layer of increasing thickness

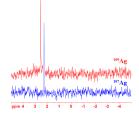


Figure: Resonance peaks of  $^{109}A_g$  and  $^{107}A_\sigma$ 

Wide resonance peaks for isospin half-integer elements



Figure: Ruderman - Kittel - Kasuya - Yosida

#### Summary

Introduction

From General Hamiltonian of many atoms:

$$H = \underbrace{\sum_{i} \frac{p_{i}^{2}}{2\mu_{i}} + V_{p-e}(r_{i})}_{On \ site} + \underbrace{\sum_{i} \underbrace{V_{X}(r_{i})}_{Exchange} + \underbrace{V_{e-e}(r_{i})}_{Resonant \ interaction} + \underbrace{V_{corr}(r_{i})}_{Correlations}$$
Between sites

To Heisenberg Hamiltonian:

$$\hat{H} = \textit{E}_{\textit{flat}} - \sum_{i,j} \textit{J}_{i,j} \hat{S}_i \cdot \hat{S}_j \qquad \textit{with} \qquad \textit{J}_{i,j} = 2 \int \psi_i(\textbf{r_i}) \psi_j(\textbf{r_j}) \hat{H} \psi_i(\textbf{r_j}) \psi_j(\textbf{r_i}) \mathrm{d}\textbf{r_i} \mathrm{d}\textbf{r_j}$$

To RKKY Hamiltonian:

$$\hat{H} = E_{flat} - \frac{J^2}{(g\mu_B)^2} \sum_{i,j} \chi(\mathbf{r_{i,j}}) \hat{S}_i \cdot \hat{S}_j$$

#### Summary

Introduction

$$\begin{split} \chi_2(r,T) &= -\frac{m}{2\pi\hbar^2} k_F^2 \left[ J_0(k_F r) Y_0(k_F r) + J_1(k_F r) Y_1(k_F r) \right. \\ &\left. - \frac{\pi^2}{12} \left( \frac{T}{T_F} \right)^2 k_F r \left( J_1(k_F r) Y_0(k_F r) + J_0(k_F r) Y_1(k_F r) \right) \right] \end{split}$$

Comparison of 2D Integrated response functions for different temperatures

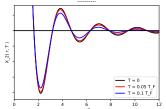


Figure: RKKY analytical response function in two dimensions

Validity Range of Sommerfeld Expansion with Respect to Temperature

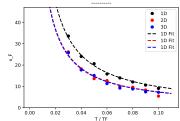


Figure: Validity range of RKKY response function under Sommerfeld's expansion

Basics of Quantum Mechanics Atomic Model Heisenberg Model

# Summary

Introduction

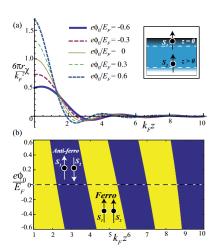
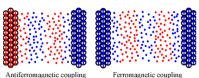


Figure: Giant Magneto-resistance in a 30A thick NiFeRu layer

#### Exchange Coupling via Transition Metals: Universal Oscillations



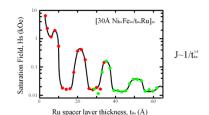


Figure: Left: RKKY susceptibility between two particles at two different interfaces with two insulators

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