Lecture note Magnetism (7)

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Lat week, we show that a ferromagnetic exchange interaction appears in Heitler-London approximation though a hopping of electrons between the sites cases anti-ferromagnetic exchange interaction. The exchange interaction due to the transfer of electrons is a kind of **kinetic exchange interaction**, which often gives anti-ferromagnetic interaction though not always [*1]. Also, we found that the spin-spin interaction is always anti-ferromagnetic in a pure two-atom-model [*2]. From the numerical simulations so far, they have found no realistic example in which the direct exchange interaction causes ferromagnetism. However we extracted the concept of direct exchange interaction from the HL approximation and inferred that some "exchange interaction" is working in any magnetic materials. We thus introduced Heisenberg Hamiltonian (Heisenberg model). You may wonder why this kind of change in the related freedoms is possible. This can be understood in the context of quantum entanglement as stated in Appendix 7A. In the appendix, it is shown that the quantum entanglement is not a pure mathematical notion but a real physical phenomenon, useful in the experiment.

4.1.3 Hubbard model

The mechanism of anti-ferromagnetic exchange interaction in electron transfer can also be seen in the following simple model. Let us consider two sites (i, j) and write the electronic states as $|n; m\rangle$ (";" separates the parameters of two states). Electron hopping between the two sites is taken into account and the hopping operator is written as $t(a_{i\sigma}^{\dagger} a_{j\sigma} + \text{h.c.})$. Due to the Pauli's exclusion principle, two electrons occupying a single site are limited to spin up-down pair. Such states have higher energy due to the on-site repulsion and can exist as intermediate states during hopping process. We write this increase in the energy in the intermediate states as U, namely

$$U = E(|0; \sigma, -\sigma\rangle) - E(|\sigma; -\sigma\rangle). \tag{4.19}$$

The hopping process, however decreases the energy in the second perturbation and the amplitude of decrease is about $|t|^2/U$. The above simple model is called **Hubbard model**, in which the hopping amplitude with the nearest neighbor is t and the electron gets on-site repulsion U for double occupation. Here we introduce the simplest two-site model but extended ones are one of the most important model in exploration of magnetism. With the notation $n_{i\sigma} = a_{i\sigma}^{\dagger} a_{i\sigma}$, the model can be expressed in Hamiltonian form as

$$\mathscr{H} = t \sum_{\sigma=\uparrow\downarrow} (a_{1\sigma}^{\dagger} a_{2\sigma} + a_{2\sigma}^{\dagger} a_{1\sigma}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}). \tag{4.20}$$

We limit the electron number as $n_{\text{e}} = 2$ then the available states are

$$|\uparrow\downarrow; 0\rangle, \; |0; \uparrow\downarrow\rangle, \; |\uparrow; \uparrow\rangle, \; \frac{1}{\sqrt{2}}(|\uparrow; \downarrow\rangle + |\downarrow; \uparrow\rangle), \; |\downarrow; \downarrow\rangle, \; \frac{1}{\sqrt{2}}(|\uparrow; \downarrow\rangle - |\downarrow; \uparrow\rangle). \tag{4.21}$$

The operators of spin at each site, total spin, and total electron number, are defined as

$$\boldsymbol{s}_i = \sum_{\sigma\sigma'} a_{i\sigma}^{\dagger} \left(\frac{\boldsymbol{\sigma}}{2}\right)_{\sigma\sigma'} a_{i\sigma'}, \quad \boldsymbol{S} = \sum_{i=1,2} \boldsymbol{s}_i, \quad N = \sum_{i,\sigma} n_{i\sigma}, \tag{4.22}$$

[*1] Superexchange interaction, which we will see in the next section, is also a kind of kinetic exchange interaction. But sometimes it gives ferromagnetic interaction[1, 2].

[*2] Then you might ask how about the Hund's rule? This is a natural question long been addressed. Actually many textbooks on the physical chemistry say that "Hund's rule is empirical rules that cannot be mathematically proved." In large scale numerical calculations, it turned out that the disturbance of nuclear-potential screening by core electrons has larger effect than the Pauli exclusion principle. This is an example and there are various new findings[3, 4]. Anyway we need more study in this field.

No.	S	S_z	E	Eigenstate
1	0	0	U	$\frac{1}{\sqrt{2}}(|\uparrow\downarrow;0\rangle - |0;\uparrow\downarrow\rangle)$
2			$\left(1+\frac{1}{a}\right)\frac{U}{2}$	$\frac{\sqrt{1+a}}{2}(|\uparrow\downarrow;0\rangle + |0;\uparrow\downarrow\rangle) + \sqrt{\frac{1-a}{2}}\,|0,0\rangle$
3			$\left(1-\frac{1}{a}\right)\frac{U}{2}$	$\sqrt{\frac{1+a}{2}}\,|0,0\rangle - \frac{\sqrt{1-a}}{2}(|\uparrow\downarrow;0\rangle + |0;\uparrow\downarrow\rangle)$
4	1	+1	0	$|1,+1\rangle$
5		0		$|1,0\rangle$
6		−1		$|1,-1\rangle$

Tab. 4.1 Eigenenergies of two-electron, two-site Hubbard model eq. (4.20). a is defined as $a^{-2} = 1 + (4t/U)^2$.

which commute with $\mathscr{H}$ and $\boldsymbol{S}^2$, S_z, N can be good quantum numbers. For $N = 2$, we can compose 6 eigenstates common for these operators from (4.21). The eigenergies of them are listed in Tab. 4.1 with definition of $a^{-2} = 1 + (4t/U)^2$. When the Coulomb repulsion is sufficiently larger than the hopping effect $t/U \ll 1$, from this table and from calculation similar to that for the direct exchange interaction, the effective spin Hamiltonian is obtained as

$$\mathscr{H}_{\text{eff}} = -J\left(\boldsymbol{s}_1 \cdot \boldsymbol{s}_2 - \frac{1}{4}\right), \quad J = -\frac{4t^2}{U}, \tag{4.23}$$

which again gives an anti-ferromagnetic exchange interaction.

4.2   Superexchange interaction

There are many magnetic materials, in which negative ions (anions) with closed shell electronic structures exists between magnetic positive ions. Figure 4.1(a) shows the crystal structure of perovskite-type $KFeF_3$, which is an anti-ferromagnet with the Néel temperature (explained later) 173 K. In the structure, F^{-1}'s exist between Fe^{2+}'s The interaction mechanism between such magnetic ions was proposed long time ago as **superexchange interaction**. As named, it is a kind of exchange interaction. In the starting point, the negative ions do not have spin and the exchange effect first causes spins in negative ions and then the created spins have interactions with magnetic ions. Hence the effect should be second order perturbation. Figure 4.1(b) shows the model, in which a part of electrons shift from a negative ion to neighboring magnetic ions. The transfer results in the appearance of a little spin on the negative ion that has the exchange interactions with neighboring magnetic ions.
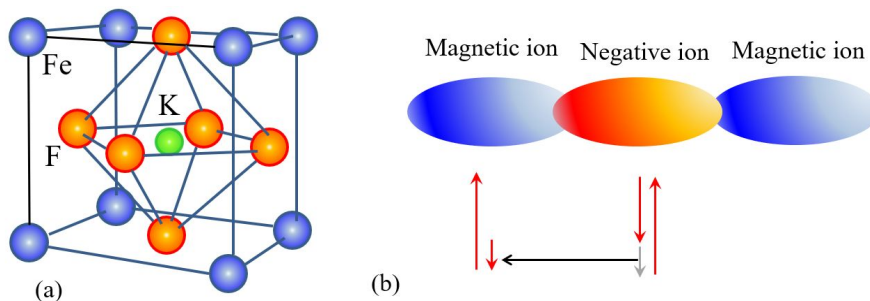

Fig. 4.1   (a) Cristal structure of anti-ferromagnet $KFeF_4$ in perovskite structure. (b) Schematic diagram of superexchange interaction.

The unperturbed state of negative ions is symmetric for spins, but the hopping to the magnetic ions is asymmetric due to the asymmetry of the magnetic ions. Hence a spin created on a negative ion reflects the direction of spin on the magnetic ion. The exchange interaction of this created spin with another magnetic ion thus results in the effective exchange interaction between magnetic ions. The above exchange interaction mechanism mediated by non-magnetic negative ions is called superexchange interaction[5].

4.2.1 Conditional change in sign and amplitude

Though the superexchange is a kind of kinetic exchange interaction, it is not necessarily anti-ferromagnetic because it is a three site problem[*3]. The sign and the amplitude of the superexchange interaction depend on the conditions such as coupling angle of magnetic ion-negative ion-magnetic ion. The dependence was half-empirically summarized as **Goodenough-Kanamori's rules**.

Consider the combination of d-orbital (i, j), and write the interaction as

$$-\sum_{i,j} 2 J_{\text{eff}}(i,j) \boldsymbol{s}_i \cdot \boldsymbol{s}_j. \tag{4.24}$$

For simplicity, we assume Hund's rule on each magnetic ion, namely the total spin $\boldsymbol{S}_1 = \sum_i \boldsymbol{s}_{1i}$, $\boldsymbol{S}_2 = \sum_j \boldsymbol{s}_{2j}$ is maximized. Let n be the number of electrons in the open shell of each ion, then $\boldsymbol{s}_i = \boldsymbol{S}/n$. The interaction is written again as in the form

$$-2 J_{12} \boldsymbol{S}_1 \cdot \boldsymbol{S}_2. \tag{4.25}$$

The half empirical rules on the amplitude and the sign are called Goodenough-Kanamori's rules[6, 7]. Here I just quote what Kanamori himself describe: (after telling the difficulty in the calculation of J_{12}) "However, about the amplitude and the sign of J_{12}, rather vague rules exist, which can be theoretically explained and show good agreements with experiments[8]."

For example, when two magnetic ions and an anion line up in a straight line, the interaction between magnetic ions of the same species is anti-ferromagnetic ($J < 0$). When one of d orbitals has electrons more than 5 and less than 5
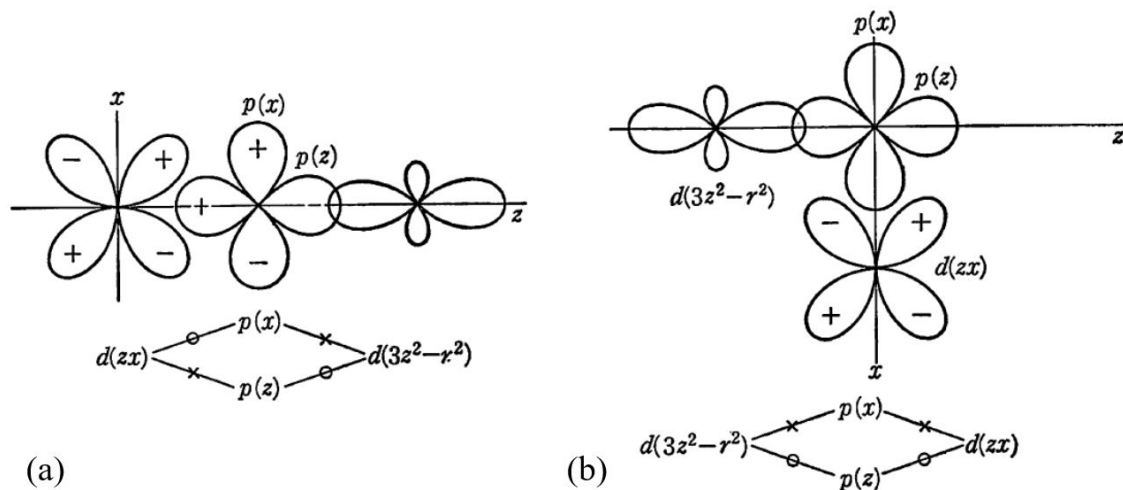

Fig. 4.2 Examples of Goodenough-Kanamori's rules. (a) Magnetic ions and an anion line up in a straight line ($180°$). (b) Bonding bends at an anion by $90°$. $+$. $-$ represent the signs of orbitals (phases). The line diagrams below the orbital drawings show electron hoppings between the orbitals. ○'s and ×'s represent possibilities of hoppings. From [8].

[*3] Conversely, the two involved interaction is anti-ferromagnetic, the total interaction should be ferromagnetic.

in the other, the interaction is ferromagnetic ($J > 0$). When the arrangement has a $90°$ bending at an anion as in (b), the tendency is inverse to (a), namely the interaction is ferromagnetic for the same species magnetic ions but the case of d^5. However there are various cases and exceptions. For details, refer to the original paper by Kanamori[7], or review articles[5].

4.3   s-d exchange interaction

In the superexchange interaction, we have considered insulating crystals without conduction electrons. Here on the contrary, consider the case of metallic crystals with many conduction electrons which interact with the spins on magnetic ions. Such situation occurs, e.g., small amount of magnetic ions like Fe or Mn are doped as impurities into non-magnetic metals.

4.3.1   Conduction electrons around local moments

Let S be the total spin operator of a magnetic impurity, s be the spin operators of conduction electrons. We write the matrix element of electron scattering by the local moment as

$$\mathcal{H}_{\text{scatt}} = -2J_{\boldsymbol{kk'}}\boldsymbol{S}\cdot\boldsymbol{s}. \tag{4.26}$$

In the long wavelength approximation ($2\pi/k$ is longer than the radius of scattering center), $J_{\boldsymbol{kk'}} = J$ (const.). In other words, the interaction is δ-function (point-contact) type and with taking the position of impurity at the origin $\boldsymbol{r} = \boldsymbol{0}$ the above is approximated by

$$\mathcal{H}_{\text{scatt}} = -2J\delta(\boldsymbol{r})\boldsymbol{S}\cdot\boldsymbol{s}. \tag{4.27}$$

We represent the conduction electrons as s, localized electrons at magnetic ion as d and call the interaction **s-d exchange interaction**. I hope we can have time to go into a many body effect caused by this interaction later. From the conduction electrons, the interaction in eq. (4.27) is equivalent to the δ-function like effective magnetic field $2J\boldsymbol{S}\delta(\boldsymbol{r})/(g_{\text{e}}\mu_{\text{B}})$ at the origin with the direction of $\boldsymbol{S}$. The Fourier transform of the field is

$$\boldsymbol{B}_{\text{eff}}(\boldsymbol{r}) = \frac{2J\delta(\boldsymbol{r})}{g_{\text{e}}\mu_{\boldsymbol{B}}}\cdot\boldsymbol{S} = \int\frac{d\boldsymbol{q}}{(2\pi)^3\sqrt{V}}\boldsymbol{B}_{\boldsymbol{q}}e^{i\boldsymbol{q}\cdot\boldsymbol{r}}. \tag{4.28}$$

We write the magnetization of conduction electrons as $\boldsymbol{m}(\boldsymbol{r})$ and the susceptibility $\chi(\boldsymbol{q})$ in the wavenumber space is defined by

$$\boldsymbol{m}(\boldsymbol{r}) = \int\chi(\boldsymbol{q})\boldsymbol{B}_{\boldsymbol{q}}\frac{d\boldsymbol{q}}{(2\pi)^3\sqrt{V}}. \tag{4.29}$$

For simplicity we consider the free electron model. We treat eq. (4.27) as a perturbation to the plane wave to obtain

$$\varphi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{V}} \pm \frac{JS}{V}\int\frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{E(\boldsymbol{k}+\boldsymbol{q})-E(\boldsymbol{k})}\frac{d\boldsymbol{q}}{(2\pi)^3\sqrt{V}}, \tag{4.30}$$

where the double sign $\pm$ reflects the sign of the inner product of $\boldsymbol{S}$ and $\boldsymbol{s}$. Then we can write

$$\boldsymbol{m}_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{g_{\text{e}}\mu_{\text{B}}}{2}(\varphi_{\boldsymbol{k}-}^*\varphi_{\boldsymbol{k}-} - \varphi_{\boldsymbol{k}+}^*\varphi_{\boldsymbol{k}+}) = -\frac{g_{\text{e}}\mu_{\text{B}}JS}{V^2}\int\left(\frac{1}{E(\boldsymbol{k}+\boldsymbol{q})-E(\boldsymbol{k})} + \frac{1}{E(\boldsymbol{k}-\boldsymbol{q})-E(\boldsymbol{k})}\right)e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\frac{d\boldsymbol{q}}{(2\pi)^3}. \tag{4.31}$$

With summing up the above over $\boldsymbol{k}$ and from eq. (4.28), (4.28), we reach the expression

$$\begin{aligned}\chi(\boldsymbol{q}) &= \frac{g_{\text{e}}^2\mu_{\text{B}}^2}{2V}\int_{k\leq k_{\text{F}}}\left(\frac{1}{E(\boldsymbol{k}+\boldsymbol{q})-E(\boldsymbol{k})} + \frac{1}{E(\boldsymbol{k}-\boldsymbol{q})-E(\boldsymbol{k})}\right)\frac{d\boldsymbol{k}}{(2\pi)^3}\\ &= \frac{3N}{8}\frac{(g_{\text{e}}\mu_{\text{B}})^2}{E_{\text{F}}}\frac{1}{2}\left(1 + \frac{4k_{\text{F}}^2-q^2}{4qk_{\text{F}}}\log\left|\frac{2k_{\text{F}}+q}{2k_{\text{F}}-q}\right|\right).\end{aligned} \tag{4.32}$$
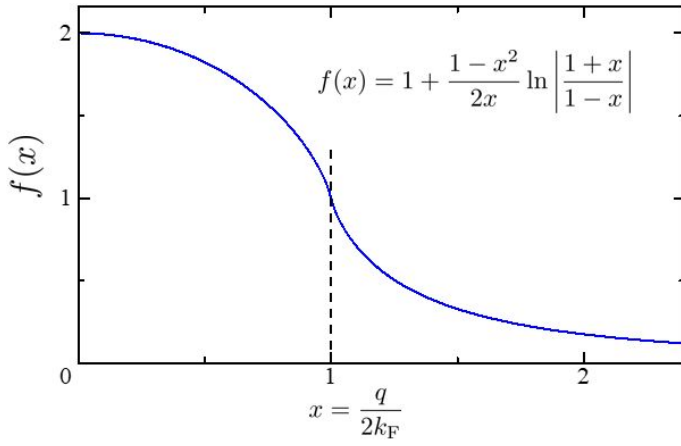
Fig. 4.3 Plot of $f(x)$ in eq. (4.33). The region is limited to $x > 0$ as $f(x)$ is an even function.

The last part in the parenthesis $(\cdots)$ is written as

$$f(x) = 1 + \frac{1 - x^2}{2x} \log \left| \frac{1 + x}{1 - x} \right|, \tag{4.33}$$

where $x = q/2k_F$ [*4]. The function is plotted in Fig. 4.3.

To calculate $\boldsymbol{m}(\boldsymbol{r})$ from eq. (4.29) and $\chi_{\boldsymbol{q}}$ in eq. (4.32), we need the integral

$$F(r) = \frac{1}{2\pi} \int d\boldsymbol{q} \, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} f\left(\frac{q}{2k_F}\right) = \frac{2}{r} \int_0^\infty q \sin(qr) f\left(\frac{q}{2k_F}\right) dq$$

$$= \frac{1}{r} \int_{-\infty}^\infty q \sin(qr) f\left(\frac{q}{2k_F}\right) dq. \tag{4.34}$$

In the application of partial integral, we need to apply Cauchy's principal value since df/dx diverges at $x = 1$ as shown in Fig. 4.3. We also use the identities

$$\int_{-\infty}^\infty \frac{\sin[2k_F r(1 \pm x)]}{1 \pm x} dx = \pi, \quad \int_{-\infty}^\infty \frac{\cos[2k_F r(1 \pm x)]}{1 \pm x} dx = 0, \tag{4.35}$$

to obtain

$$F(r) = -16\pi k_F^3 \frac{2k_F r \cos(2k_F r) - \sin(2k_F r)}{(2k_F r)^4}. \tag{4.36}$$

Then we finally reach the expression of the local magnetization $\boldsymbol{m}(\boldsymbol{r})$:

$$\boldsymbol{m}(\boldsymbol{r}) = -\frac{3}{32\pi^2} \frac{N g_e \mu_B F(r) J}{E_F} S_z, \tag{4.37}$$

where we take z-direction to that of $\boldsymbol{S}$ and the expectation value S_z is used.

4.3.2 RKKY interaction

In eq. (4.37), the dependence on r is from $F(r)$ in eq. (4.36), the r-dependent part of which is plotted in Fig. 4.4. The decay with r is associated with an oscillation.

If we have another magnetic ion within the decay length, the conduction electrons interact with it by s-d exchange interaction and as a result, a kind of exchange interaction between the magnetic ions is established. This is called **RKKY interaction** [*5]. The interaction is estimated as

$$-\int \boldsymbol{m}(\boldsymbol{r}) \boldsymbol{B}_{\text{eff}}(\boldsymbol{r} - \boldsymbol{R}) d\boldsymbol{r} = \frac{3N}{16\pi^2} \frac{J^2}{E_F} F(R) S_{1z} S_{2z}, \tag{4.38}$$

[*4] The notation is confusing with the Fermi distribution function (the function itself is close!). But we do not have so many good symbols and this is a custom notation.

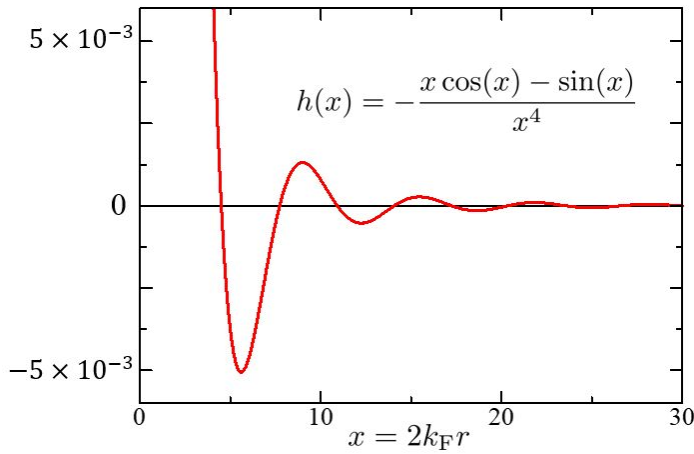[*5] Capital letters of Ruderman-Kittel-Kasuya-Yosida [9, 10, 11].

Fig. 4.4 Plot of r-dependent part of eq. (4.36), that is $-(x \cos x - \sin x)x^4$ ($x = 2k_{\mathrm{F}}r$). It decays with r to zero with an oscillation.

where $\boldsymbol{R}$ is the vector connecting the two magnetic ions, and the spins of them are written as $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$. This equation is obtained from the expectation value $\boldsymbol{m}(\boldsymbol{r})$ and thus expressed in the product of expectation values along z-axis. It is an exchange interaction and we can replace $S_{1z}S_{2z}$ with $\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$ to modify it to an RKKY Hamiltonian for quantum mechanical calculations.

As in eq. (4.38), the RKKY interaction oscillates with the period about $(2k_{\mathrm{F}})^{-1}$ and decays as R^{-3}. However when the distance between the ions is short, namely the second ion is close to the origin in Fig. 4.4, the interaction between the ions is always ferromagnetic because the s-d interaction works twice. De Gennes pointed out the possibility of ferromagnetism in diluted magnetic alloys[12] via this RKKY ferromagnetic interaction. However it is still unclear weather such systems really exist or not.

4.4   Double exchange interaction

The **double exchange interaction** mechanism was proposed by Zener[13] for the explanation of ferromagnetism in Mn perovskite type compound magnets. A typical example is aMnO$_3$, which is an insulating anti-ferromagnet due to the superexchange interaction. However, with replacing a part of La with Ca, the material $La_{1-x}Ca_xMnO_3$ ($0.2 < x < 0.4$) shows metallic conduction and transits to a ferromagnet.

Such a system can be modelized as Fig. 4.5. $3d$ electron levels are split by the octahedral potential of perovskite to t_{2g} orbitals and e_g orbitals. t_{2g} orbitals have lower energy and strongly localized while e_g orbitals spread over the neighbors, being hybridized with $2s$, $2p$ orbitals to form a band. In LaMnO$_3$, each Mn ion is 3+ and in the high spin state with a single electron in an e_g orbital. In spite of the formation of a band, the system is an insulator because of the on-site Coulomb repulsion U for the hopping to the neighboring e_g orbitals (due to the anti-ferromagnetic order, the electron spins do not disturb the hopping). The situation is close to the Hubbard model introduced in Sec. 4.1.3, and such insulators caused by the electron correlation are called **Mott insulators**.
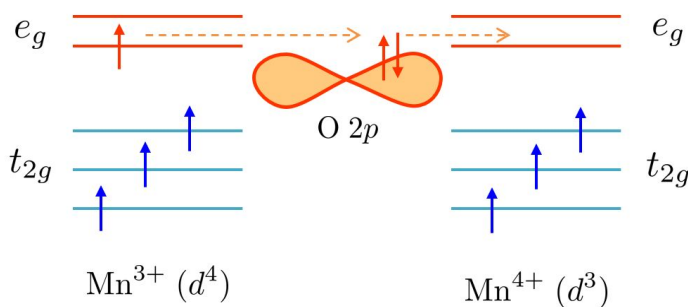

Fig. 4.5 Schematic diagram of double exchange interaction.

With replacing a part of La(3+) with Ca(2+), a part of electrons in Mn is transferred to Ca resulting in the appearance of Mn^{4+}. In Mn^{4+}, the e_g orbital is empty making the transfer of electrons via oxygen atoms possible (sometimes described as "hole doping" in the vocabulary of semiconductor physics). This leads to the breaking of electron correlation that sustains the insulating manner and the metallic conduction appears. In the metallic state, when an e_g electron shifts to the next Mn ion, the energy is lower for aligned spins of t_{2g} electrons due to Hund's rule in ions. And the higher transfer of electrons causes lowering of the kinetic energy resulting in the ferromagnetism. As can be seen in the above scenario, this can also be viewed as a kinetic exchange interaction.

So far we have seen superexchange, RKKY, and double exchange interactions. At the first glance they are so different, but it is difficult to say weather they are essentially different. The naming of the interactions comes from the human wish to understand the complicated behavior of spins in simple views. It is at a higher level than the fundamental law of physics and sticking to the classification of interactions is not a meaningful idea. Particularly in the case of spins, the interaction is due to the magic of entanglement as in Appendix 7A. We must keep in mind that sometimes the magic goes away.

4.5   Anisotropic exchange interaction

In many cases actual electrons in crystals have anisotropy reflecting complicated band structures. Such anisotropies in orbitals are reflected to spins through the spin-orbit interactions. Hence in treating the exchange interactions, we should take into account the anisotropy. We thus express the exchange interaction between sites i and j with a tensor $\boldsymbol{J}_{ij}$. Then the Hamiltonian of the spin system is given by

$$\mathscr{H} = \sum_j \mathscr{H}_A(\boldsymbol{S}_j) - \frac{1}{2}\sum_{i \neq j} {}^t\boldsymbol{S}_i \boldsymbol{J}_{ij} \boldsymbol{S}_j, \tag{4.39}$$

where ${}^t\boldsymbol{a}$ is the transpose of $\boldsymbol{a}$. The anisotropic energy on site is written as $\mathscr{H}_A$. We write the tensor elements indices as $J_{ij}^{\mu\nu}$ and separate (μ, ν) to symmetric and anti-symmetric parts as

$$J^{\mu\nu} = \frac{1}{2}[(J^{\mu\nu} + J^{\nu\mu}) + (J^{\mu\nu} - J^{\nu\mu})] \equiv K^{\mu\nu} + \sum_{\xi=x,y,z} \epsilon_{\mu\nu\xi} D^{\xi}. \tag{4.40}$$

$\epsilon_{\mu\nu\xi}$ is the complete anti-symmetric tensor (Levi=Chivita symbol). The site indices (i,j) are omitted. The second term in the rhs, the anti-symmetric part of eq. (4.39) is expressed as

$$\mathscr{H}_{ij}^{(DM)} = {}^t\boldsymbol{S}_i \left\{ \sum_{\xi} \epsilon_{\mu\nu\xi} D_{ij}^{\xi} \right\} \boldsymbol{S}_j = \boldsymbol{D}_{ij} \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_j). \tag{4.41}$$

$\boldsymbol{D}_{ij} = -\boldsymbol{D}_{ji}$ and this anti-symmetric exchange interaction $\mathscr{H}_{ij}^{(DM)}$ is called **Dzyaloshinskii-Moriya** (DM) interaction[14, 15].

The DM interaction is important in the discussion of magnetic anisotropy of anti-ferromagnets, weak ferromagnets. In resent researches, the DM interaction is important in the magnetic interaction between thin films and in other spintronics field.

Chapter 5
Theories of magnetic insulators
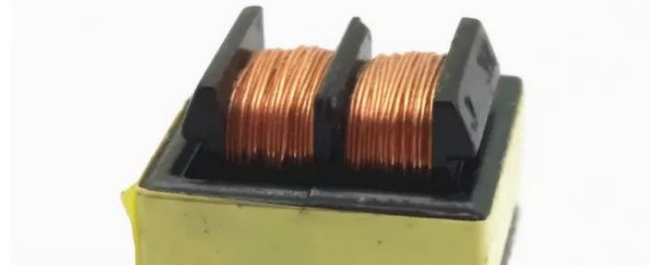
Ferrite core transformer

There are many magnetic insulators as **ferrites** (AFe_2O_4, A=Mn, Co, Ni, Cu, Zn, $\cdots$). They are very advantageous for the high frequency use in the absence of eddy current and of skin effect. Now they are indispensable in high frequency techniques. Also since they do not deteriorate such as rust, the ferrites are mostly used for the magnets on blackboards etc., the magnetic sheets that can be used with cut [*6]

In the previous chapter we have introduced the Heisenberg model, which is one of the human-friendly models for dealing with magnetism. In insulators, superexchange interactions work between localized spins, and a situation close to the Heisenberg model may be realized in essence. Here we will see what kind of phenomena the model includes.

5.1 Molecular field theory

We consider **mean field theory**, which is the most basic approach in many body problems. In the field of magnetism, the approach is also called **molecular field approximation**.

5.1.1 Ferromagnetic Heisenberg model

We consider the Heisenberg model in eq. (4.13) with the magnetic field of magnetic flux density $\boldsymbol{B}$:

$$\mathscr{H} = -2J\sum_{\langle i,j\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \mu\sum_i \boldsymbol{B}\cdot\boldsymbol{S}_i, \tag{5.1}$$

where the sum on $\langle i,j\rangle$ is taken for the nearest neighbors. The interaction is ferromagnetic, i.e., $J > 0$, μ is taken as positive. In the mean field approximation for site i, the surrounding spins are replaced with averaged magnetic moments.

$$\mathscr{H}_{\text{eff}}(i) = -2J\sum_{\delta} \langle \boldsymbol{S}_{i+\delta}\rangle \cdot \boldsymbol{S}_i - \mu\boldsymbol{B}\cdot\boldsymbol{S}_i = -\mu\boldsymbol{B}_{\text{eff}}\cdot\boldsymbol{S}_i. \tag{5.2}$$

δ is for nearest neighbors. The effective field $\boldsymbol{B}_{\text{eff}}$ in eq. (5.2):

$$\mu\boldsymbol{B}_{\text{eff}} = 2J\sum_{\delta} \langle \boldsymbol{S}_{i+\delta}\rangle + \mu\boldsymbol{B}, \tag{5.3}$$

which is also called molecular field.

[*6] Long time ago, the ferrites were also used in magnetic tapes.

Here we use the expression (2.51) for magnetization M per single ion with replacing $g_J\mu_B \to \mu$, $J \to S$, Brillouin function $B_J \to B_S$ to obtain

$$M = \mu S B_S \left[\frac{\mu S}{k_B T} \left(B + \frac{2\alpha_z J}{\mu^2} M \right) \right]. \tag{5.4}$$

α_z is the number of neighboring sites and the direction of $\boldsymbol{B}$ is taken to z-direction. Equation (5.4) is a self-consistent equation for M.

We use the expansion of coth in Brillouin function B_S and obtain

$$B_S(x) = \frac{S+1}{3S}x - \frac{1}{90}\frac{[(S+1)^2 + S^2](S+1)}{S^3}x^3 + \cdots. \tag{5.5}$$

Then eq. (5.4) is expanded as

$$\left(1 - \frac{2\alpha_z J}{\mu^2}\chi_0\right) M + \frac{1}{90}[(S+1)^2 + S^2]\frac{1}{(k_B T)^3}\left(\frac{2\alpha_z J}{\mu^2}\right)^2 M^3 = \chi_0 B. \tag{5.6}$$

$\chi_0 = \mu^2 S(S+1)/3k_B T$ represents the Curie law in eq. (2.53).

When (5.6) has a non-zero solution of M (spontaneous magnetization) for $B = 0$, the system can have a ferromagnetic state. The condition is the coefficient of the first order in M in the lhs of (5.6) becomes zero. This gives the ferromagnetic transition temperature (**Curie temperature**) T_C as

$$k_B T_C = \frac{2}{3}S(S+1)\alpha_z J. \tag{5.7}$$

The susceptibility for $T > T_C$ is obtained from eq. (5.6) by considering the first order term as

$$\chi = \chi_0 \left(1 - \frac{2\alpha_z J}{\mu^2}\chi_0\right)^{-1} = \mu^2 \frac{S(S+1)}{3k_B(T - T_C)}, \tag{5.8}$$

which diverges as $(T - T_C)^{-1}$. This behavior is called **Curie-Weiss law**.

Appendix 7A: Quantum entanglement and quantum dot experiments

Although the magnetic-mediated spin-to-spin interaction is very weak, we found that a strong spin-to-spin interaction occurs due to the relationship with the orbit. Then the spin Hamiltonian model is introduced. As above, in quantum theory, the freedoms in an interaction model can be exchanged under some conditions. This is on the concept of **quantum entanglement**, which is widely used in the quantum information field.

7A.1   Quantum entanglement and effective Hamiltonian

The readers are already familiar with the concept and here a brief introduction is given. Let us consider two systems with two-dimensional orthogonal basis $\{|1\rangle, |2\rangle\}$ and $\{|p\rangle, |q\rangle\}$. We write the wavefunctions in the systems as $|\psi\rangle = a_1 |1\rangle + a_2 |2\rangle$, $|\phi\rangle = a_p |p\rangle + a_q |q\rangle$. When these two have no relation between them, a state of the combined system (of course the combined system can be considered even if there are no relation) is written as a direct product of the two wavefunctions:

$$|\Psi_n\rangle = |\psi\rangle \otimes |\phi\rangle = a_1 a_p |1\rangle |p\rangle + a_1 a_q |1\rangle |q\rangle + a_2 a_p |2\rangle |p\rangle + a_2 a_q |2\rangle |q\rangle. \tag{7A.1}$$

On the other hand, we consider the case when the wavefunction of combined system is written in the form

$$|\xi\rangle = (|1\rangle |p\rangle + |2\rangle |q\rangle)/\sqrt{2}. \tag{7A.2}$$

In this state, assume we perform measurement on $|\psi\rangle$ and obtain e.g. the result 1. Then without observation on $|\phi\rangle$ and without direct interaction between the two systems, the state of $|\phi\rangle$ is determined to p by the above measurement. This situation is described as $|\psi\rangle$ and $|\phi\rangle$ are **entangled**. This was clearly pointed out in the famous EPR paper[16, 17]. In particular the state in eq. (7A.2) is called a maximally entangled state and the operations on the systems are unseparable.

Further, we write another maximally entangled state

$$|\zeta\rangle = (|1\rangle |q\rangle + |2\rangle |p\rangle)/\sqrt{2}, \tag{7A.3}$$

and consider the case the basis space is limited to $\{|\xi\rangle, |\zeta\rangle\}$. We assume the Hamiltonian in the system $\{|1\rangle, |2\rangle\}$

$$\mathscr{H}_{\mathrm{n}} = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix}. \tag{7A.4}$$

Then

$$\langle \xi | \mathscr{H}_{\mathrm{n}} | \xi \rangle = h_{11} + h_{22}, \quad \langle \xi | \mathscr{H}_{\mathrm{n}} | \zeta \rangle = h_{12} + h_{21}, \quad \langle \zeta | \mathscr{H}_{\mathrm{n}} | \zeta \rangle = h_{11} + h_{22}. \tag{7A.5}$$

Hence if we can prepare an operator $\mathscr{H}_{\mathrm{a}}$ working on $\{|p\rangle, |q\rangle\}$ and gives the same matrix as $\mathscr{H}_{\mathrm{n}}$

$$\mathscr{H}_{\mathrm{a}} = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix}, \tag{7A.6}$$

$\mathscr{H}_{\mathrm{n}}$ and $\mathscr{H}_{\mathrm{a}}$ give the same results in the basis space $\{|\xi\rangle, |\zeta\rangle\}$.

As seen above, the concept of "effective Hamiltonian" works when the basis space is limited to entangled states of two freedoms. In such states, operations on one system is equivalent to those on the other system. Hence they are working as "operators" very differently but equivalent. In quantum physics, though not always explicitly, the concept of quantum entanglement is used in various situations.

7A.2 Quantum entanglement and observation

Quantum entanglement is not only a tool for theory, but also used widely in experiments, confirming that the EPR paradox is not a mere thought experiment.

The electron paramagnetic resonance is introduced as an experiment to observe the Larmor precession of spins in magnetic field. The traditional way to detect the resonance is to detect the lowering in the Q-value of resonator due to the absorption of energy in electromagnetic wave by the spin system at the resonance. To give a change in the characteristics of a macroscopic resonator, an ordinary experiment in microwave needs at least 10^{10} spins[18]. In this method, in other words, the magnetic field caused by the magnetic dipoles of spins are detected though the interaction in eq. (4.1). The signal is naturally tiny and it is hopeless to detect single spin precession.

Let us consider "what is measurement." A possible answer is that a measurement is to create an entanglement between the freedoms of an object and those of something human can directly distinguish. As a system for measurement we consider $\{|\uparrow\rangle, |\downarrow\rangle\}$ and $\{|A\rangle, |B\rangle\}$ as another system which human can directly distinguish. Then the measurement is to create a maximally entangled state

$$\Psi = \frac{1}{\sqrt{2}}[|\uparrow\rangle |A\rangle + |\downarrow\rangle |B\rangle]. \tag{7A.7}$$

The system $\{|A\rangle, |B\rangle\}$ is readily integrated out and the measurement is accomplished when this Ψ is created [*7].

Now, then, in the case of a spin, instead of entanglement of spin with a photon through the magnetic moment, entanglement with other freedom with much larger effect might make the detection of single spin possible.

(to be continued).

[*7] In the terms of Schrödinger's cat problem, dead/alive of the cat is determined before the box is opened.

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