2022.5.25 Lecture 7

10:25 – 11:55

Lecture on

Magnetic Properties of Materials

磁性 (Magnetism)

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Review

1. Landau diamagnetism
2. de Haas-van Alphen effect
3. Orbital diamagnetism of graphene, graphite

Chapter 4 Interaction between spins

1. Exchange interaction from Heitler-London approximation

Outline

Spin Hamiltonian and quantum entanglement

Hubbard Hamiltonian

Superexchange interaction

RKKY interaction

Double exchange interaction

Theory of Magnetic insulators

Molecular field approximation

Spin Hamiltonian and quantum entanglement

Spin Hamiltonian for EPR analysis:

Obtained by integrating out the orbital part in the second order perturbation.

$$\tilde{\mathcal{H}} = \mu_{\mathrm{B}} \boldsymbol{S} \tilde{\boldsymbol{g}} \boldsymbol{H} + D\left[S_z^2 - \frac{S(S+1)}{3}\right] + E(S_x^2 - S_y^2)$$

Direct exchange interaction:

$$\mathscr{H}_{\mathrm{int}} = K_{ab} - \frac{1}{2} J_{ab}(1 + 4\boldsymbol{s}_a \cdot \boldsymbol{s}_b)$$

This gives the same matrix elements for the basis of relevant levels.

Quantum entanglement

Two systems, freedoms

bases $\begin{cases} \{|1\rangle, |2\rangle\} \\ \{|p\rangle, |q\rangle\} \end{cases}$

states

$$|\psi\rangle = a_1 |1\rangle + a_2 |2\rangle$$

$$|\phi\rangle = a_p |p\rangle + a_q |q\rangle$$

Not entangled:

$$|\Psi_{\mathrm{n}}\rangle = |\psi\rangle \otimes |\phi\rangle = a_1 a_p |1\rangle |p\rangle + a_1 a_q |1\rangle |q\rangle + a_2 a_p |2\rangle |p\rangle + a_2 a_q |2\rangle |q\rangle$$

The state is written as a direct product.

Maximally entangled state:

$$|\xi\rangle = \frac{1}{\sqrt{2}}(|1\rangle |p\rangle + |2\rangle |q\rangle)$$

Two states are unseparable.

Quantum entanglement and effective Hamiltonian

Maximally entangled state: $|\xi\rangle = \frac{1}{\sqrt{2}}(|1\rangle|p\rangle + |2\rangle|q\rangle)$

Another maximally entangled state: $|\zeta\rangle = \frac{1}{\sqrt{2}}(|1\rangle|q\rangle + |2\rangle|p\rangle)$

Let us consider the case the basis is limited to $\{|\xi\rangle, |\zeta\rangle\}$

Consider a Hamiltonian working on $\{|1\rangle, |2\rangle\}$ $\mathscr{H}_{\mathrm{n}} = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix}$

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

Consider a Hamiltonian working on $\{|p\rangle, |q\rangle\}$ $\mathscr{H}_{\mathrm{a}} = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix}$

Though $\mathscr{H}_{\mathrm{n}}$ and $\mathscr{H}_{\mathrm{a}}$ are completely different, as long as we limit the basis to $\{|\xi\rangle, |\zeta\rangle\}$ we cannot distinguish $\mathscr{H}_{\mathrm{n}}$ and $\mathscr{H}_{\mathrm{a}}$.

Quantum measurement and entanglement

$$N_{\min} = \frac{3k_B T V}{2\pi g^2 \mu_B^2 S(S+1) Q_0} \left(\frac{\Delta H_0}{H_0}\right) \sqrt{\frac{k_B T_d F B}{P_0}}$$

In inductive measurement the EPR needs $N_{min} \sim 10^{10}$

How you make this to one?

What is measurement?

System to be measured: $\{|\uparrow\rangle, |\downarrow\rangle\}$

Degree of freedom which human can distinguish: $\{|A\rangle, |B\rangle\}$

Measurement is to create a maximally entangled state between them.

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

Schrödinger's cat problem is a problem of measurement.

$$|\text{Alive cat}\rangle |\gamma-\rangle + |\text{Dead cat}\rangle |\gamma+\rangle$$

Coulomb blockade in quantum dots

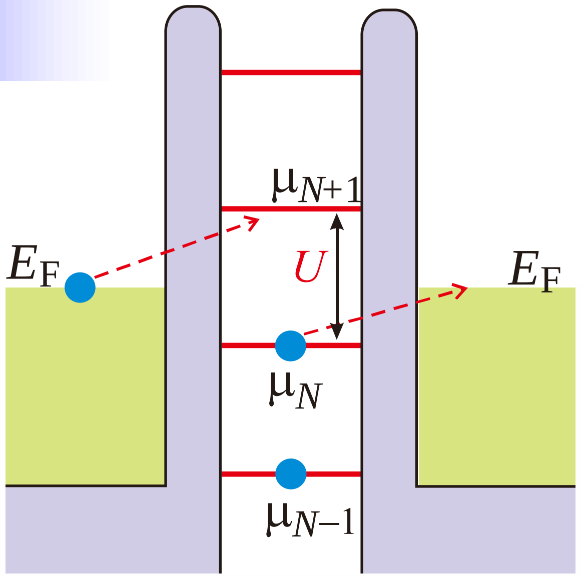
Constant interaction: U

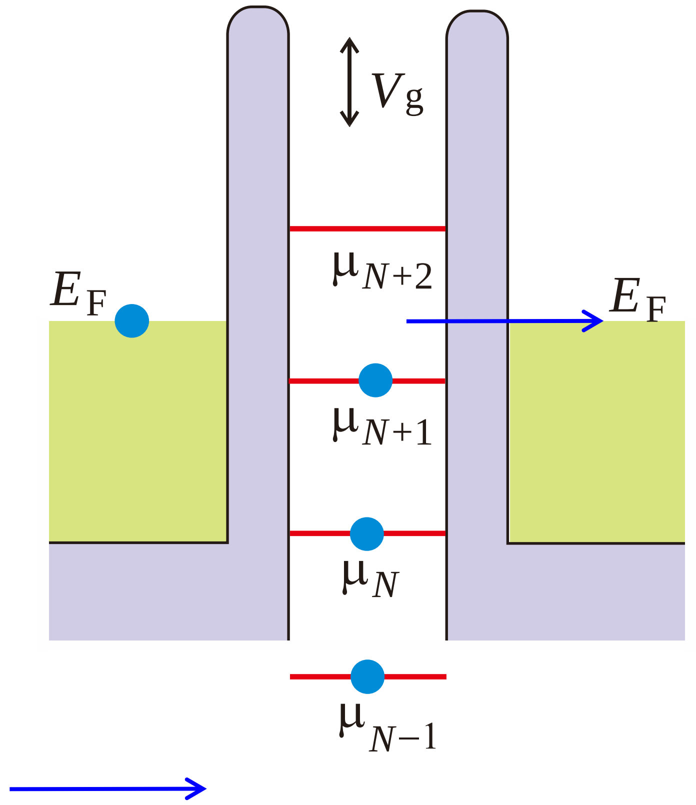
Electron number: N
Interaction energy

$$E_{cN} = {}_N C_2 U = \frac{N(N-1)U}{2} = \frac{U(N-1/2)^2}{2} - \frac{U}{8}$$

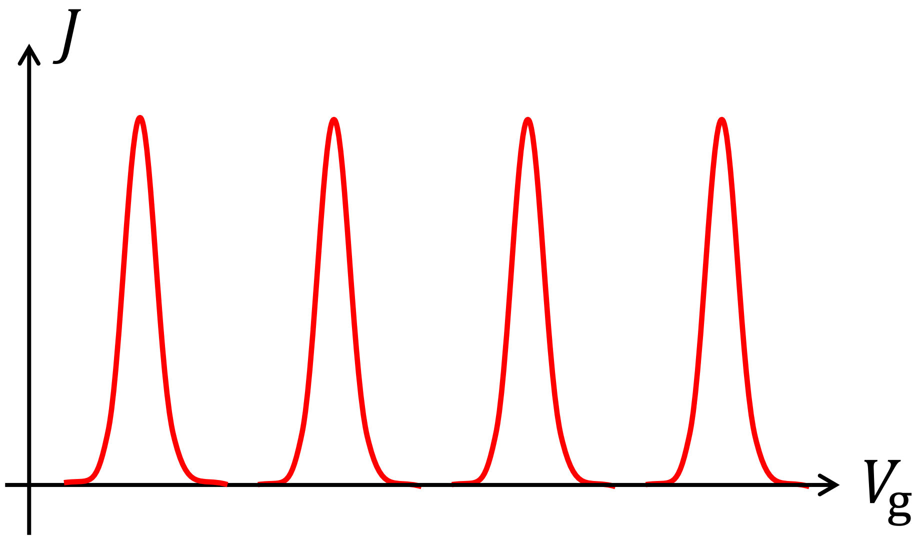
Chemical potential

$$\Delta E_+(N) = (N-1)U$$

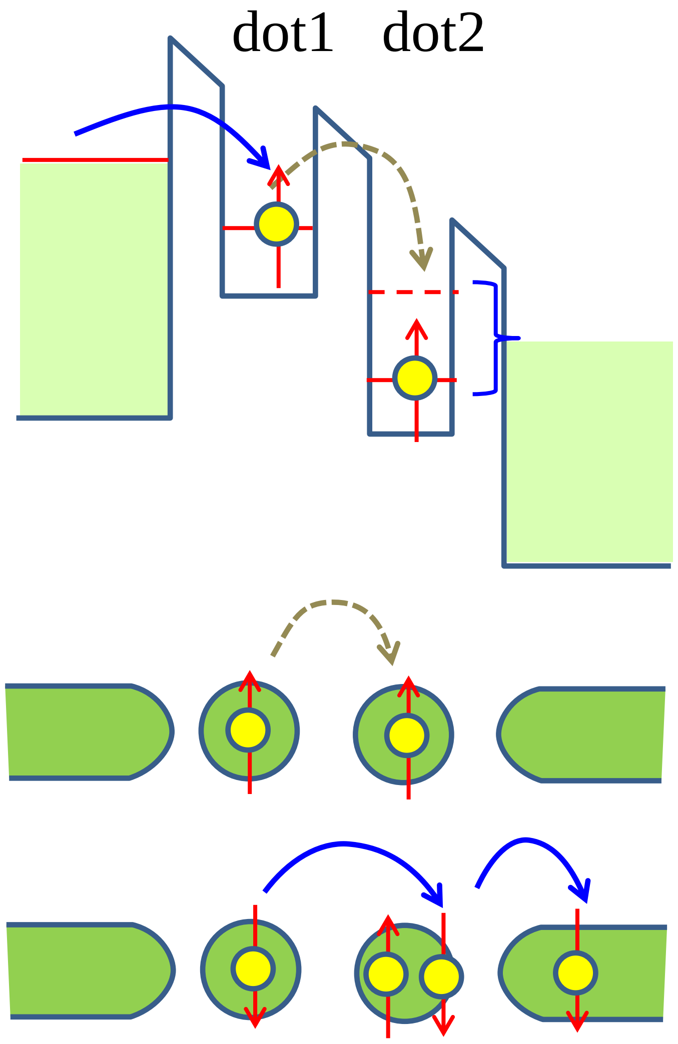




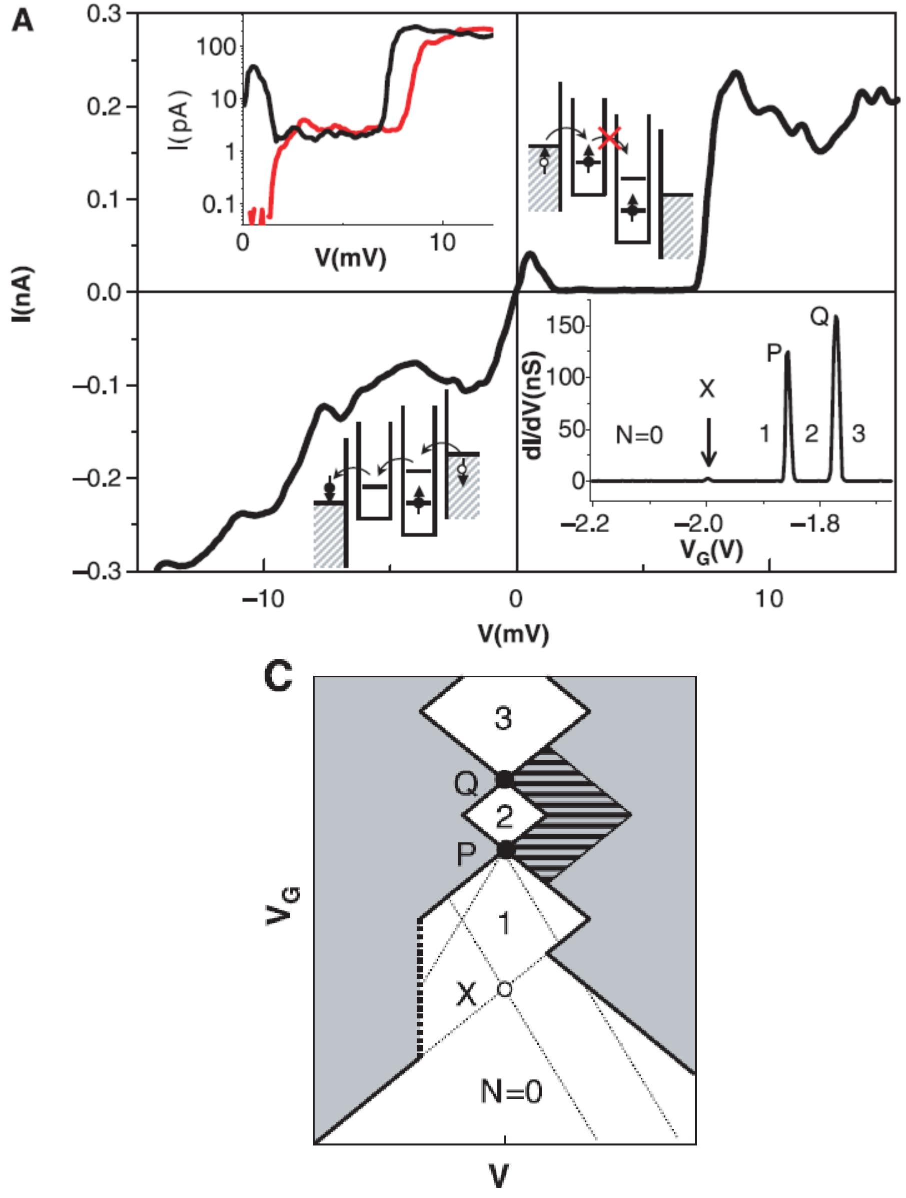
Coulomb oscillation



Pauli blockade

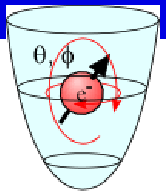


When both dot1 and dot2 are occupied by up (down) spin, the conduction is blocked.

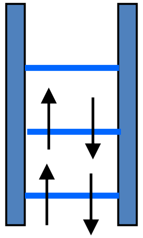


K. Ono et al., Science **297**, 1313 (2002)

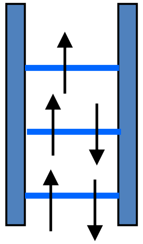
Spin quantum bit



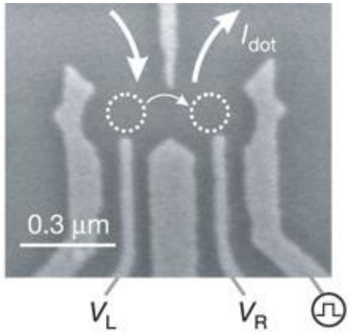
F. H. Koppens et al. Nature 442, 766 (2006)

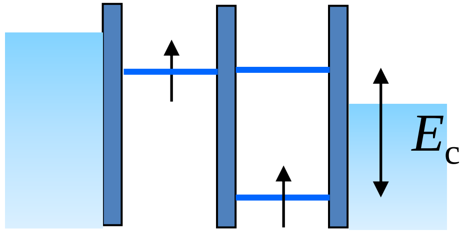


Even electron QD
No spin

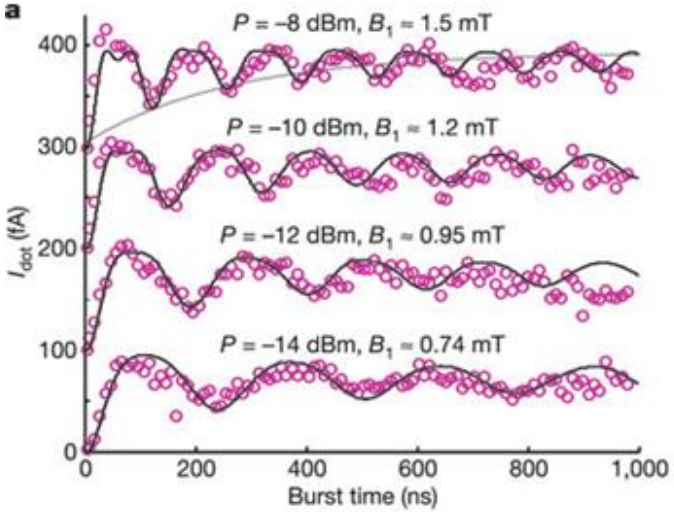


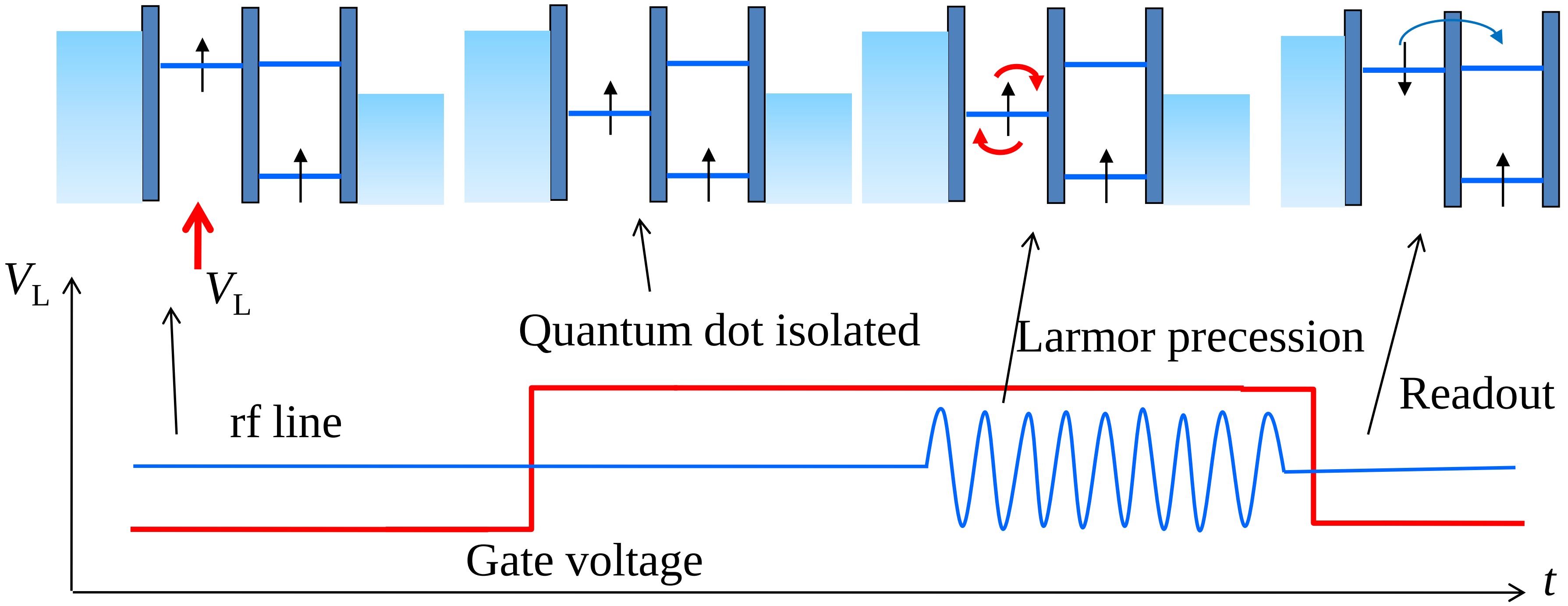
Odd electron QD
Spin 1/2





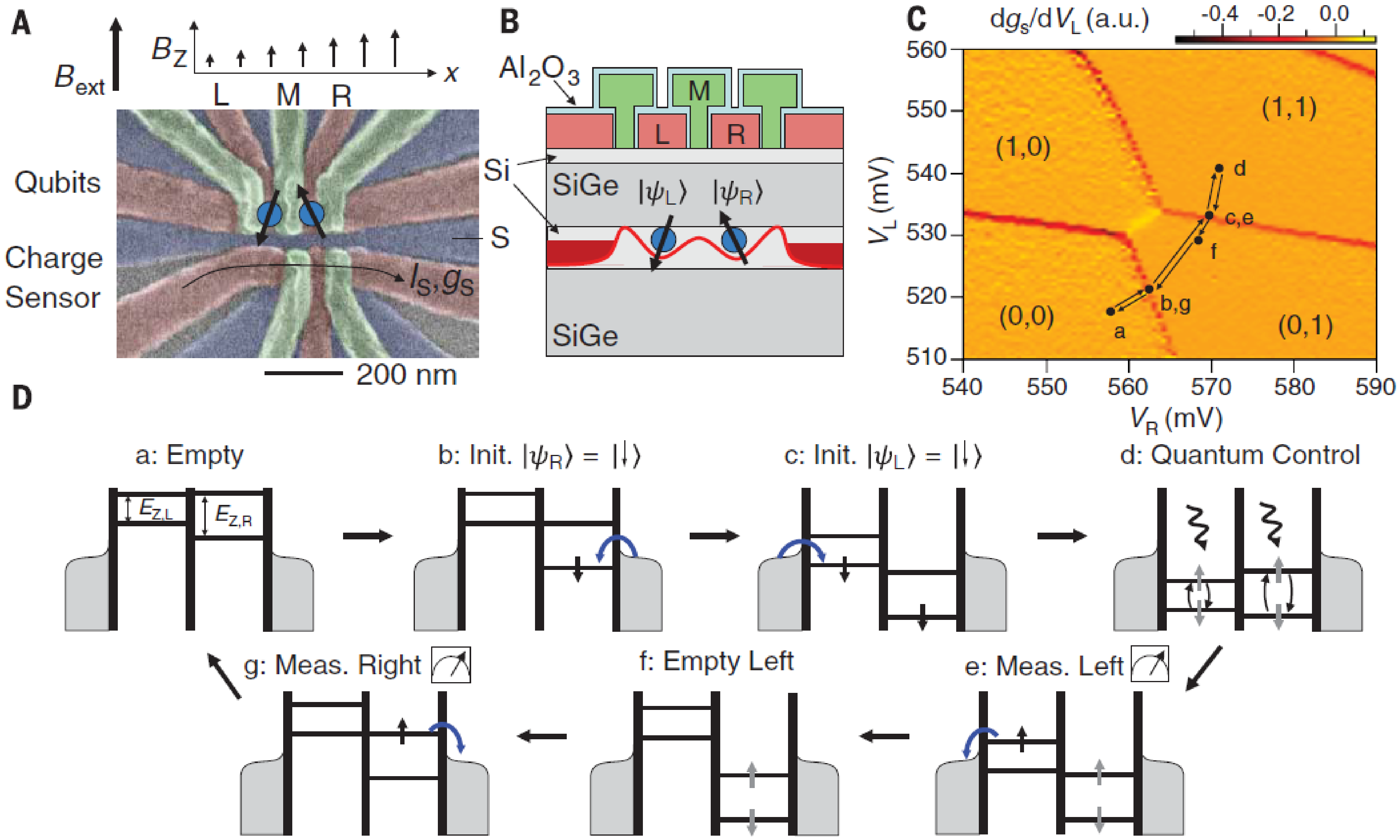
Pauli blockade



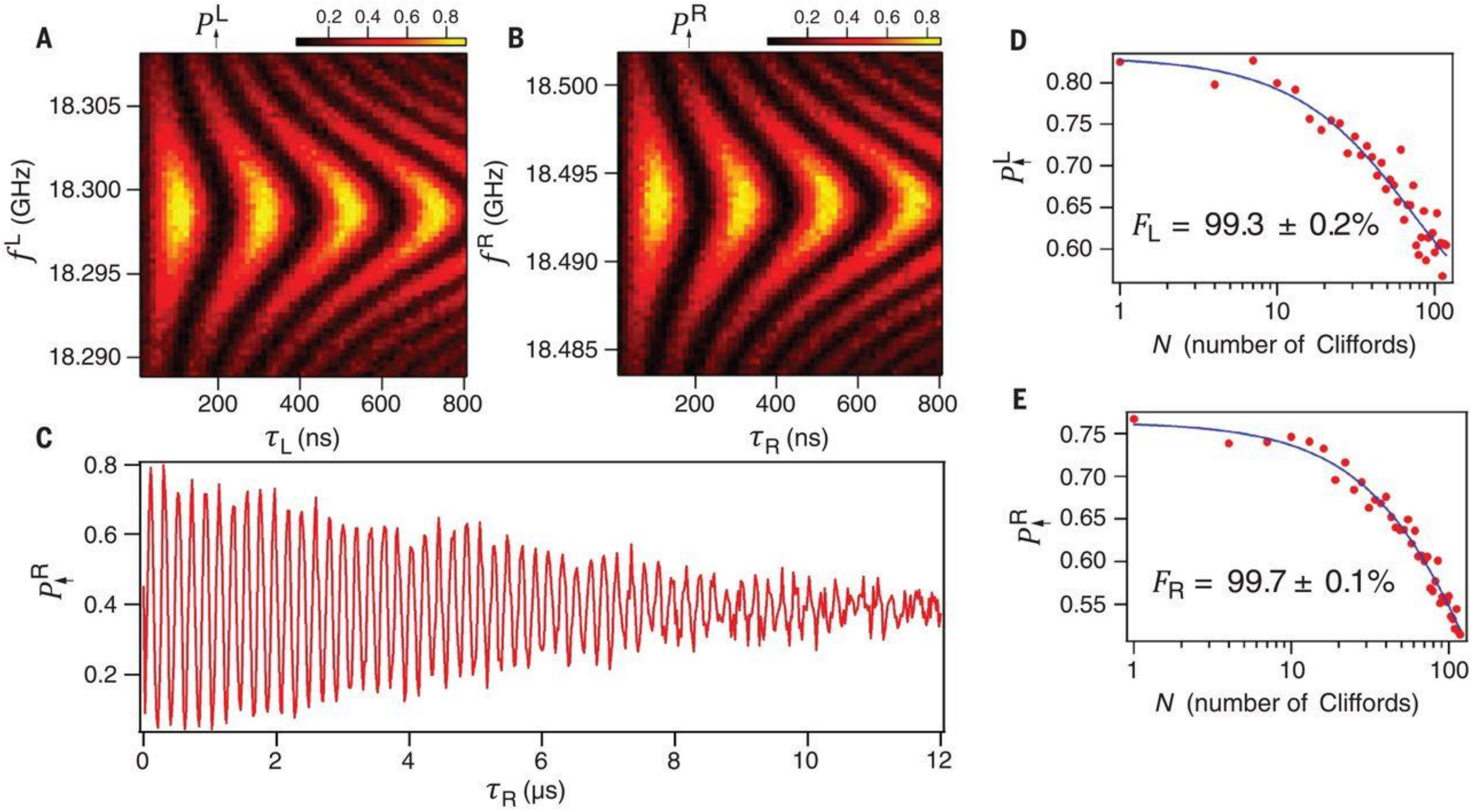


CNOT gate for electron spins

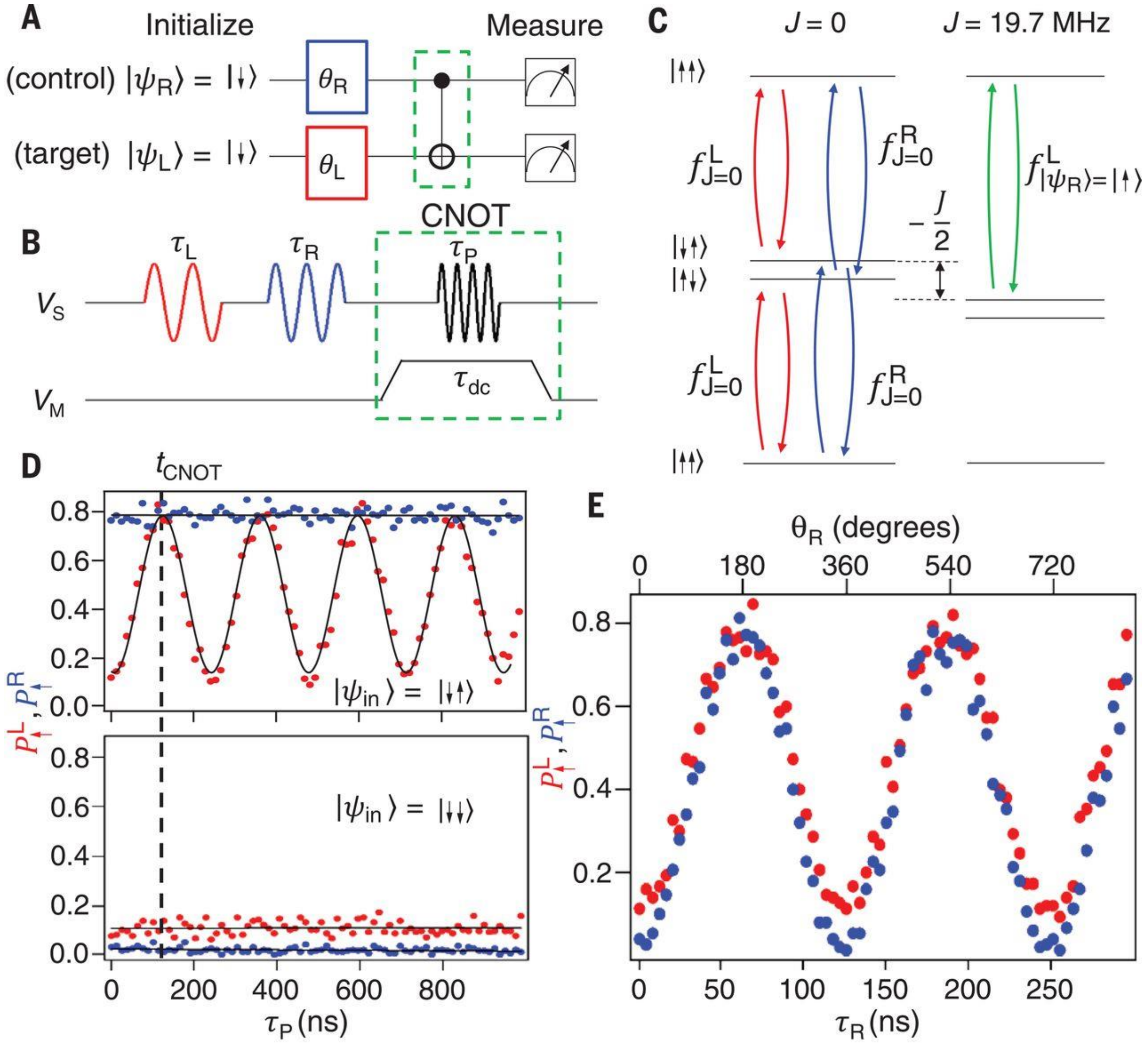
Zajac et al. Science **359**, 439 (2018).



Detection of Larmor precession



Spin-charge entanglement and detection of spin-spin interaction



Hubbard model

Anti-ferromagnetic exchange interaction by electron transfer

Two site model: (i, j)

Hopping operator: $t(a_{i\sigma}^{\dagger} a_{j\sigma} + \mathrm{h.c.})$

$$|n; m\rangle = |\sigma; -\sigma\rangle \xrightarrow{t} |0; \sigma, -\sigma\rangle \xrightarrow{t} |\sigma; -\sigma\rangle$$

Intermediate state
Enhancement U

Second perturbation energy gain

$$\frac{t^2}{U}$$

$$n_{i\sigma} = a_{i\sigma}^{\dagger} a_{i\sigma}$$

In Hamiltonian form: $$\mathscr{H} = t \sum_{\sigma=\uparrow\downarrow} (a_{1\sigma}^{\dagger} a_{2\sigma} + a_{2\sigma}^{\dagger} a_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})$$

Two-site Hubbard Hamiltonian

Effective Hamiltonian for 2-site Hubbard Hamiltonian

Possible 6-states: $|\uparrow\downarrow;0\rangle\,,\ |0;\uparrow\downarrow\rangle\,,\ |\uparrow;\uparrow\rangle\,,\ \frac{1}{\sqrt{2}}(|\uparrow;\downarrow\rangle+|\downarrow;\uparrow\rangle),\ |\downarrow;\downarrow\rangle\,,\ \frac{1}{\sqrt{2}}(|\uparrow;\downarrow\rangle-|\downarrow;\uparrow\rangle)$

Good quantum number operators

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

$$a^{-2}=1+(4t/U)^2$$

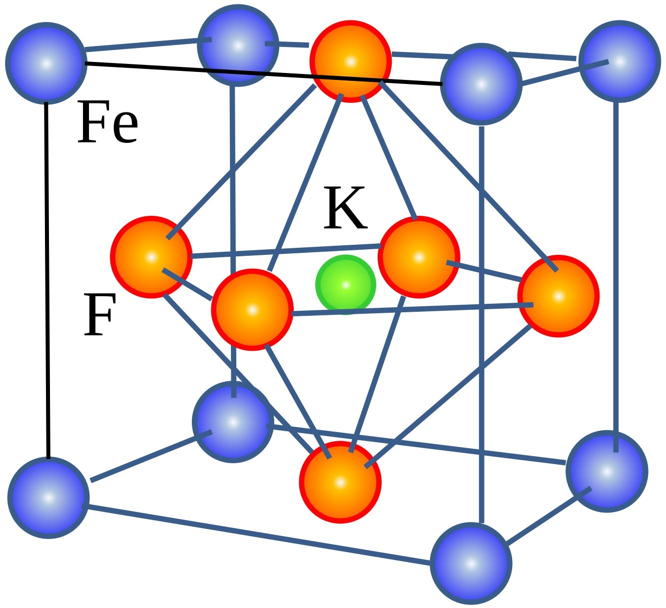
No.	S	S_z	E	Eigenstate
1	0	0	U	$\frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow;0\rangle-\lvert 0;\uparrow\downarrow\rangle)$
2			$\left(1+\frac{1}{a}\right)\frac{U}{2}$	$\frac{\sqrt{1+a}}{2}(\lvert\uparrow\downarrow;0\rangle+\lvert 0;\uparrow\downarrow\rangle)+\sqrt{\frac{1-a}{2}}\lvert 0,0\rangle$
3		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

$$\mathscr{H}_{\rm eff}=-J\left(\boldsymbol{s}_1\cdot\boldsymbol{s}_2-\frac{1}{4}\right),$$

$$J=-\frac{4t^2}{U}$$

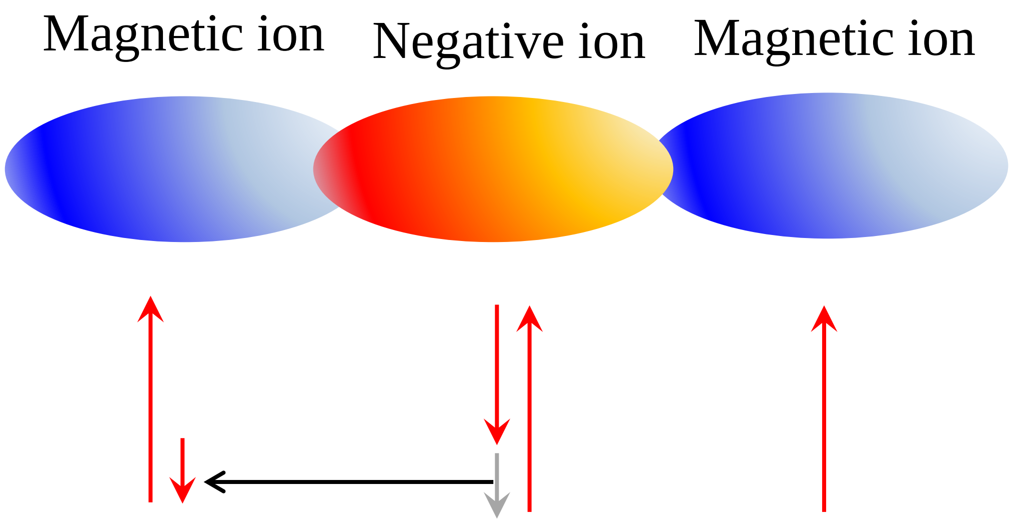
Anti-ferromagnetic

Superexchange interaction



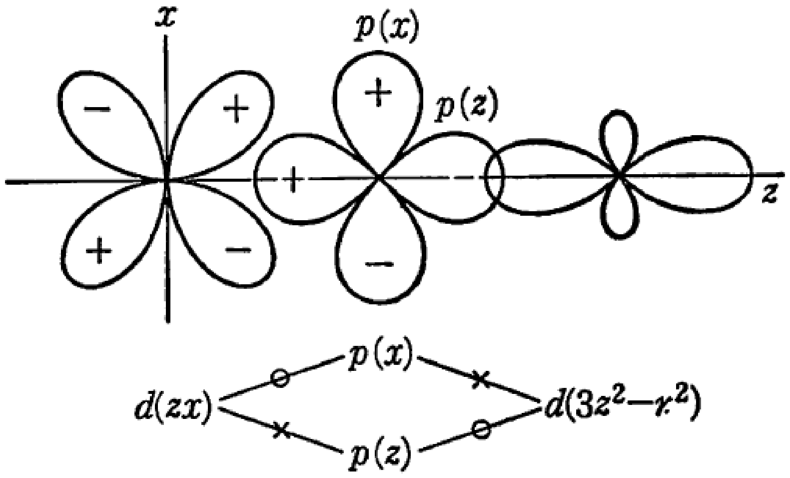
Compounds of magnetic ions and closed shell negative ions often have anti-ferromagnetism or ferromagnetism.

What is the mechanism (spin-spin interaction?) of magnetism?

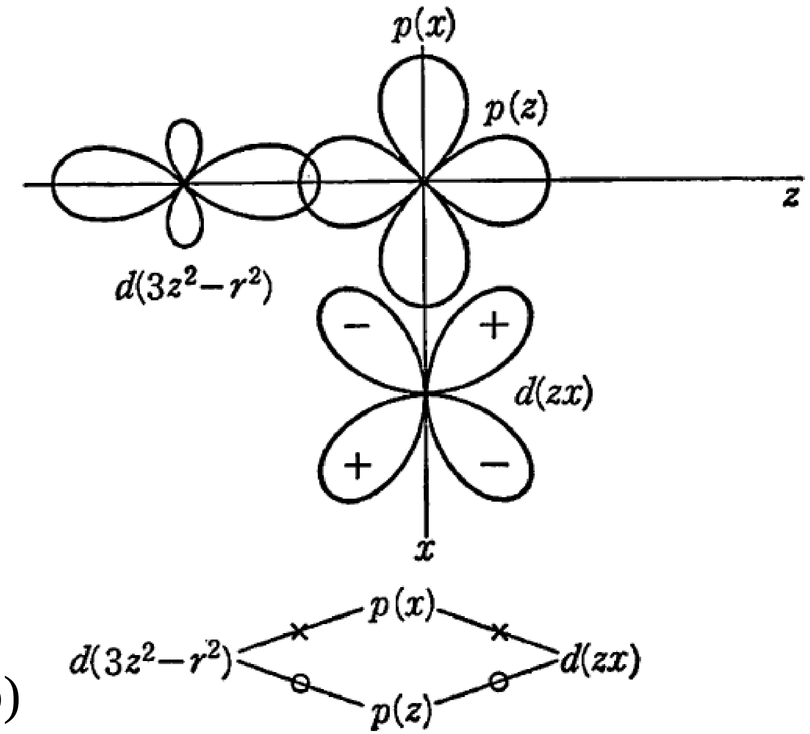


Superexchange mechanism
Small amount of electrons on a negative ions moves to a neighboring magnetic ion. Then spin appears on the negative ion which have exchange interaction with another neighboring magnetic ion.

Goodenough-Kanamori rules



(a)



(b)

Angles, orbitals, electrons numbers determine ferromagnetic, anti-ferromagnetic and the strength

s-d exchange interaction

Scattering of electrons ***s*** by a local magnetic ion ***S*** at the origin.

$$|\boldsymbol{k},\sigma\rangle \rightarrow |\boldsymbol{k}',\sigma'\rangle \qquad \mathscr{H}_{\rm scatt} = -2J\delta(\boldsymbol{r})\boldsymbol{S}\cdot\boldsymbol{s}$$

This works as if a delta-function magnetic field: $2J\boldsymbol{S}\delta(\boldsymbol{r})/(g_{\rm e}\mu_{\rm B})$

Fourier transformation:

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

Magnetic moment spatial distribution and susceptibility in frequency space.

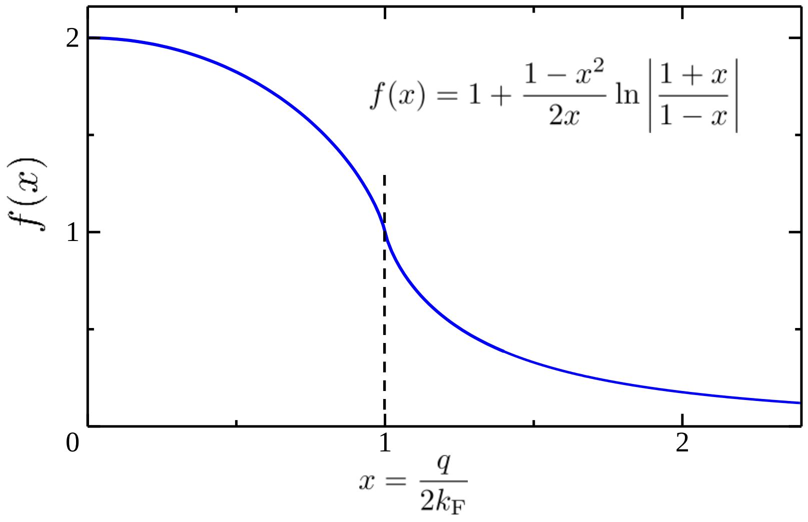
$$\boldsymbol{m}(\boldsymbol{r}) = \int\chi(\boldsymbol{q})\boldsymbol{B}_{\boldsymbol{q}}\frac{d\boldsymbol{q}}{(2\pi)^3\sqrt{V}}$$

Perturbation of $\mathscr{H}_{\rm scatt}$ on plane waves

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

$$\boldsymbol{m}_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{g_{\rm e}\mu_{\rm B}}{2}(\varphi^*_{\boldsymbol{k}-}\varphi_{\boldsymbol{k}-} - \varphi^*_{\boldsymbol{k}+}\varphi_{\boldsymbol{k}+})$$

RKKY interaction



$$\boldsymbol{m}_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{g_e\mu_B}{2}(\varphi^*_{\boldsymbol{k}-}\varphi_{\boldsymbol{k}-} - \varphi^*_{\boldsymbol{k}+}\varphi_{\boldsymbol{k}+})$$

$$= -\frac{g_e\mu_B JS}{V^2}\int\left(\frac{1}{E(\boldsymbol{k}+\boldsymbol{q})-E(\boldsymbol{k})} + \frac{1}{E(\boldsymbol{k}-\boldsymbol{q})-E(\boldsymbol{k})}\right)e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\frac{d\boldsymbol{q}}{(2\pi)^3}$$

$$\chi(\boldsymbol{q}) = \frac{g_e^2\mu_B^2}{2V}\int_{k\le k_F}\left(\frac{1}{E(\boldsymbol{k}+\boldsymbol{q})-E(\boldsymbol{k})} + \frac{1}{E(\boldsymbol{k}-\boldsymbol{q})-E(\boldsymbol{k})}\right)\frac{d\boldsymbol{k}}{(2\pi)^3}$$

$$= \frac{3N}{8}\frac{(g_e\mu_B)^2}{E_F}\frac{1}{2}\left(1 + \frac{4k_F^2 - q^2}{4qk_F}\log\left|\frac{2k_F+q}{2k_F-q}\right|\right)$$

$$x = q/2k_F \qquad f(x) = 1 + \frac{1-x^2}{2x}\log\left|\frac{1+x}{1-x}\right|$$

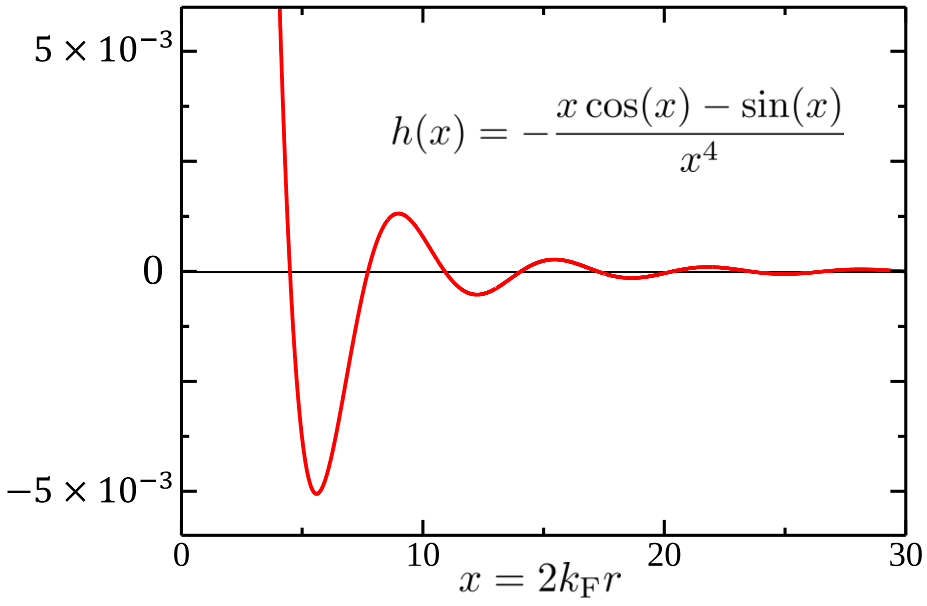
$$F(r) = \frac{1}{2\pi}\int d\boldsymbol{q}e^{i\boldsymbol{q}\cdot\boldsymbol{r}}f\left(\frac{q}{2k_F}\right) = \frac{2}{r}\int_0^\infty q\sin(qr)f\left(\frac{q}{2k_F}\right)dq$$

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

RKKY interaction (2)

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

$$F(r) = -16\pi k_\mathrm{F}^3 \frac{2k_\mathrm{F}r\cos(2k_\mathrm{F}r) - \sin(2k_\mathrm{F}r)}{(2k_\mathrm{F}r)^4}$$

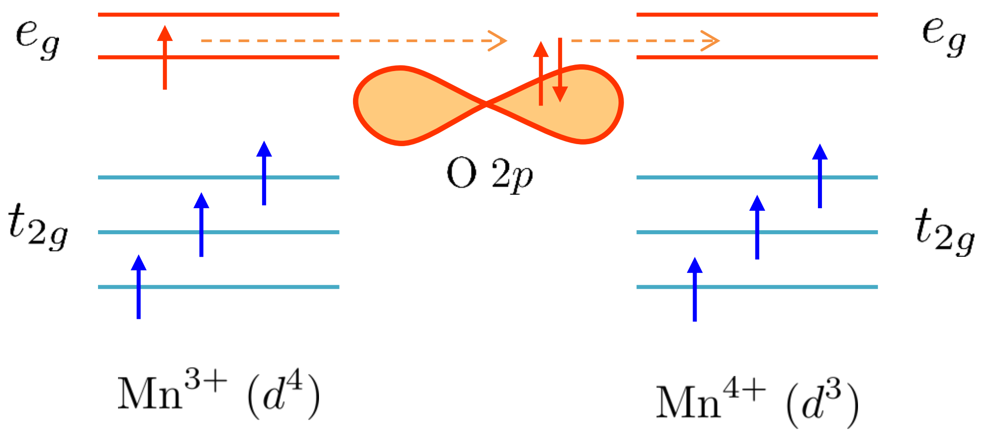


$$\boldsymbol{m}(\boldsymbol{r}) = -\frac{3}{32\pi^2}\frac{Ng_\mathrm{e}\mu_\mathrm{B}F(r)J}{E_\mathrm{F}}S_z$$

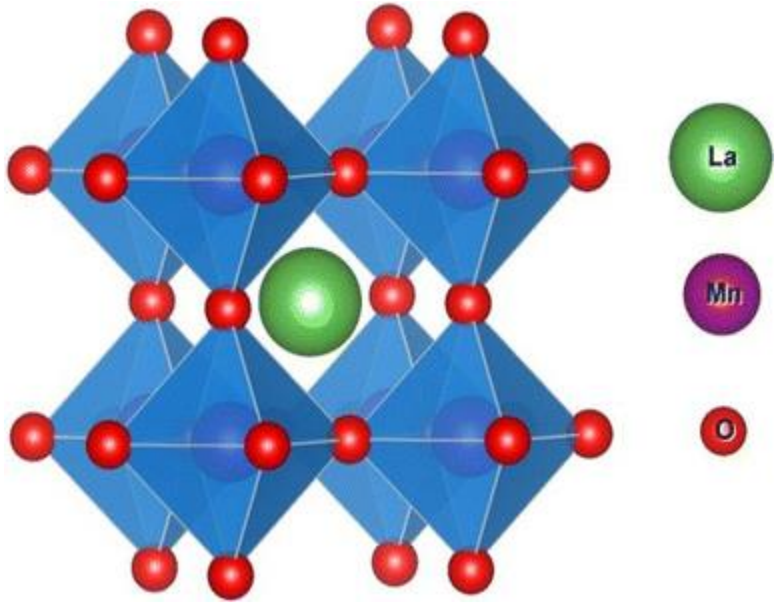
Second magnetic ion at $\boldsymbol{R}$

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

Double exchange interaction

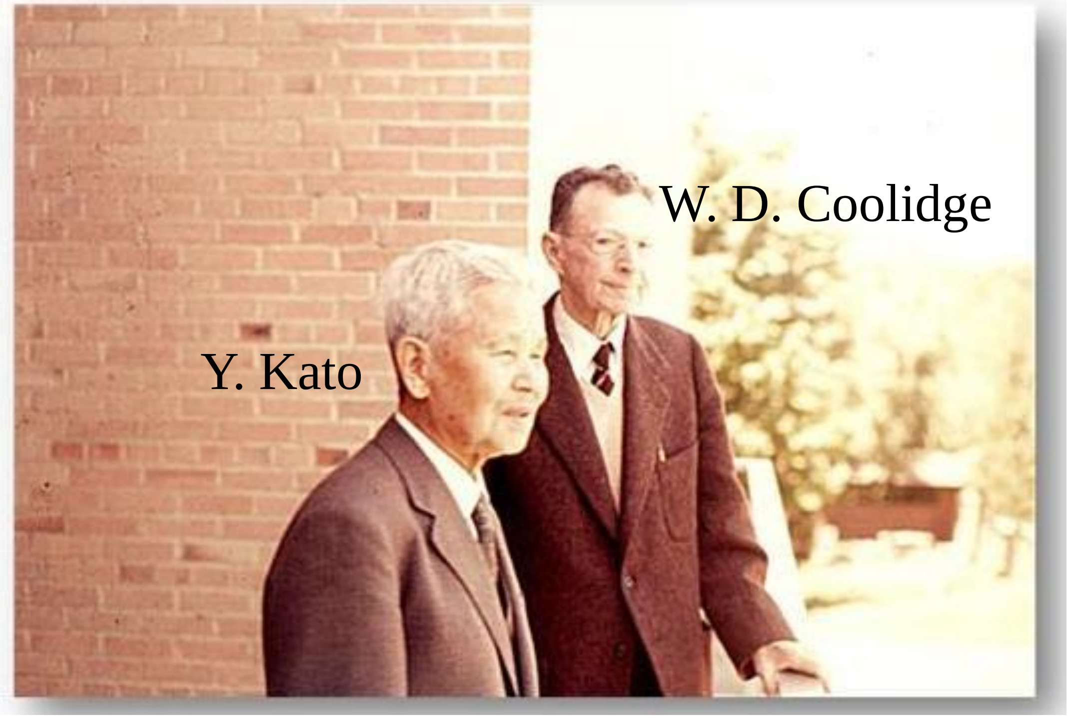


$LaMnO_3$

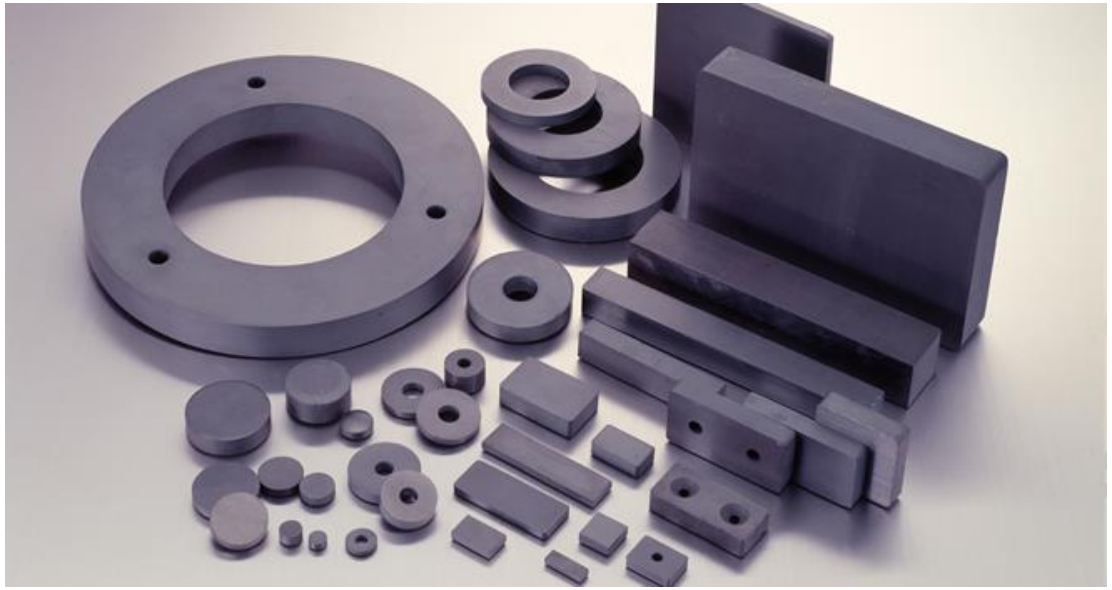


$LaMnO_3$ are anti-ferromagnetic insulator (Mott insulator). But when some La is replaced with Ca, Mn^{4+} ions appear. The system becomes metallic and at the same time this material shows ferromagnetism.

: Kind of kinetic exchange interaction.

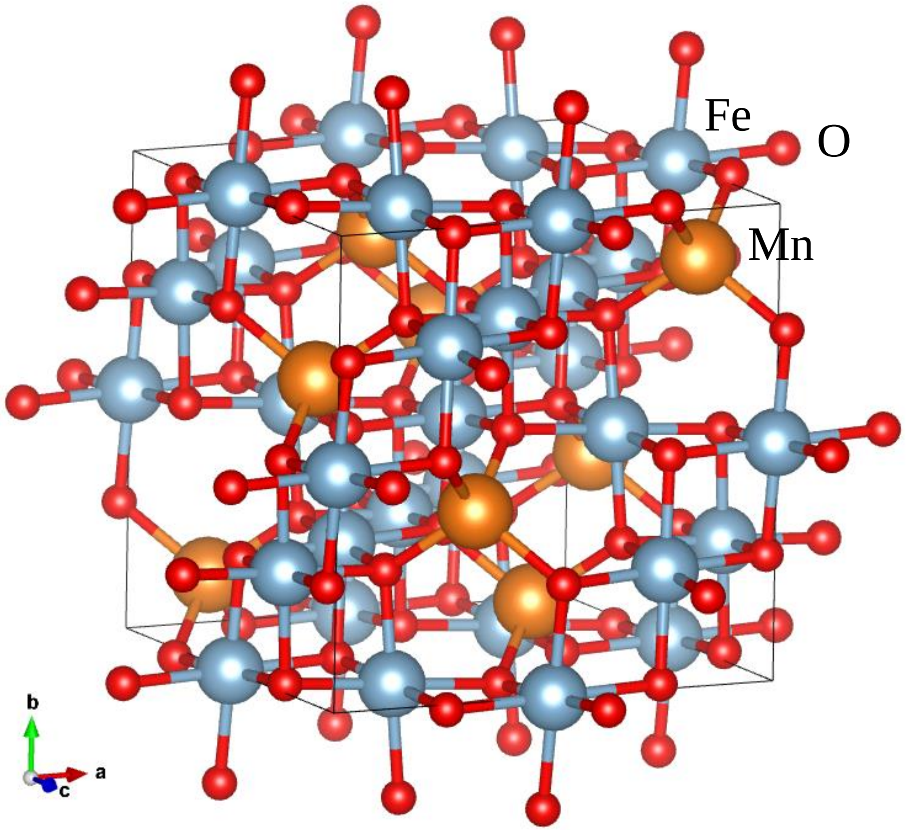


http://teetokue.air-nifty.com/blog/2008/04/59_9f47.html



Chapter 5

Theories of Magnetic Insulators



Molecular field approximation

Ferromagnetic Heisenberg Hamiltonian: $$\mathscr{H} = -2J\sum_{\langle i,j\rangle}\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \mu\sum_i \boldsymbol{B}\cdot\boldsymbol{S}_i \qquad J,\ \mu>0$$

Average field approximation:
(molecular field approximation)

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

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

Remember $M = g_J\mu_{\text{B}}JB_J\left(\frac{g_J\mu_{\text{B}}JB}{k_{\text{B}}T}\right)$ replace $g_J\mu_{\text{B}}\to\mu,\ J\to S,\ B_J\to B_S$

then $$M = \mu S B_S\left[\frac{\mu S}{k_{\text{B}}T}\left(B + \frac{2\alpha_z J}{\mu^2}M\right)\right]$$

Brillouin function is expanded as $$B_S(x) = \frac{S+1}{3S}x - \frac{1}{90}\frac{[(S+1)^2+S^2](S+1)}{S^3}x^3 + \cdots$$

Molecular field approximation (2)

then $$\left(1-\frac{2\alpha_z J}{\mu^2}\chi_0\right)M+\frac{1}{90}[(S+1)^2+S^2]\frac{1}{(k_\mathrm{B}T)^3}\left(\frac{2\alpha_z J}{\mu^2}\right)^2 M^3=\chi_0 B$$

with $$\chi_0=\mu^2 S(S+1)/3$$

The first order term drops at $k_\mathrm{B}T_\mathrm{C}=\frac{2}{3}S(S+1)\alpha_z J$ which gives the Curie temperature.

Curie-Weiss law $$\chi=\chi_0\left(1-\frac{2\alpha_z J}{\mu^2}\chi_0\right)^{-1}=\mu^2\frac{S(S+1)}{3k_\mathrm{B}(T-T_\mathrm{C})}$$

Summary

Spin Hamiltonian and quantum entanglement

Hubbard Hamiltonian

Superexchange interaction

RKKY interaction

Double exchange interaction

Theory of Magnetic insulators

Molecular field approximation