Kondo effect in multi-level and multi-valley quantum dots

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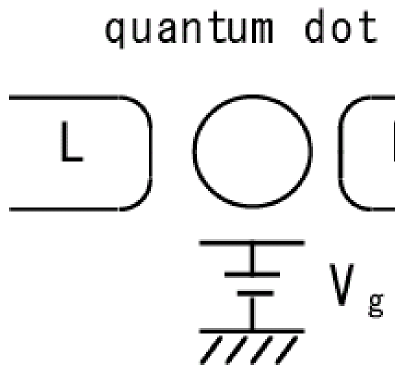
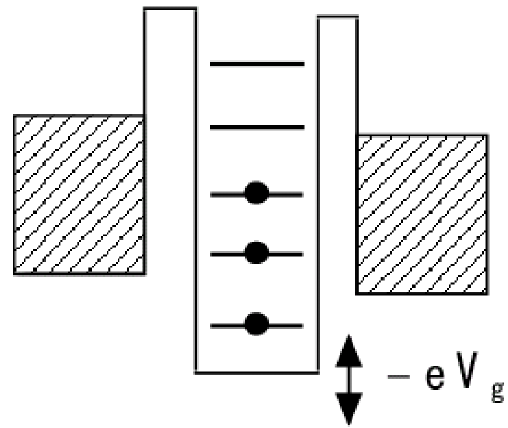
Outline

1. Introduction: next three slides for quantum dots
2. Kondo effect in quantum dots with S=1/2
   Review of Kondo physics
3. Kondo effect in multi-level quantum dots
   Experimental results
4. Theory of SU(4) Kondo effect in quantum dots
   S=1/2 and orbital degeneracy
   Evidence of the marginal fixed point
5. Kondo effect in multi-valley quantum dots
   Silicon, carbon nanotube, graphene, etc.
   New Kondo due to small exchange interaction?

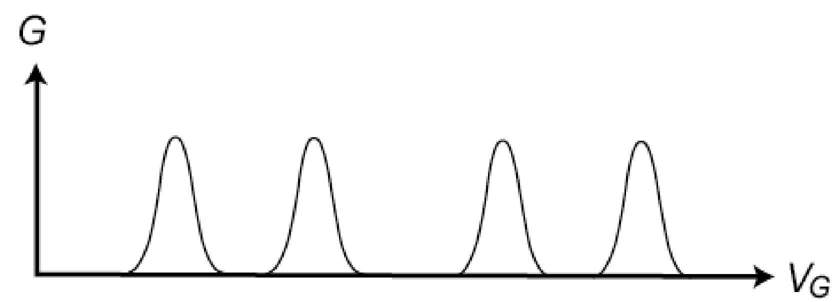
(1) Coulomb oscillation and Coulomb blockade





- Quantum dots: zero-dimensional systems of nano-meter scale
- Transport through "discrete levels" in quantum dots
- The levels are controlled by gate voltage.

→ <u>peak structure of current</u>

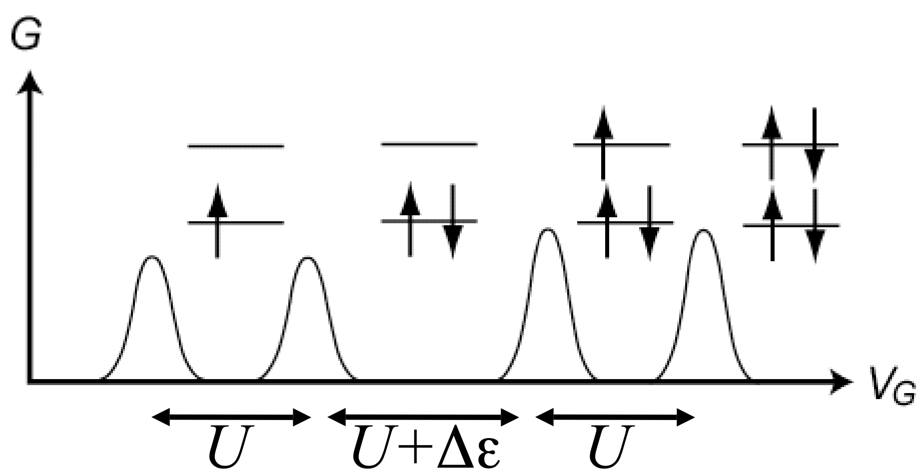


(2) Electro-chemical potential

e.g. Constant interaction model

$$E_N = \sum_{i=1}^{N} \varepsilon_i + \binom{N}{2} U = \sum_{i=1}^{N} \varepsilon_i + \frac{N(N-1)}{2} U,$$

$$\mu_N = E_N - E_{N-1} = \varepsilon_N + (N-1)U$$

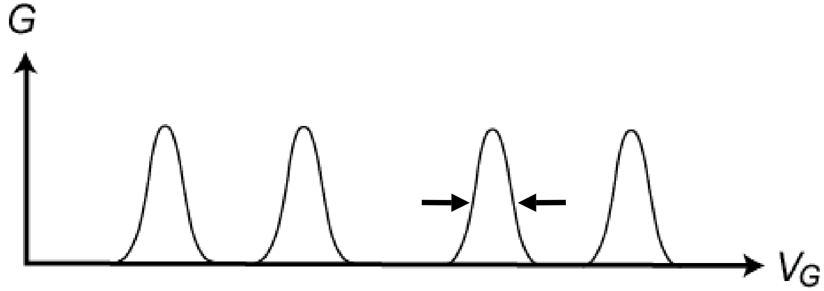


$$\mu_1 = \varepsilon_1$$
$$\mu_2 = \varepsilon_1 + U$$
$$\mu_3 = \varepsilon_2 + 2U$$
$$\mu_4 = \varepsilon_2 + 3U$$

- "Coulomb blockade" between current peaks.
- The number of electrons, *N*, is changed one by one.

(3) Condition for Coulomb oscillation and blockade

(level spacing), (Charging energy) >> $k_B T$, Γ



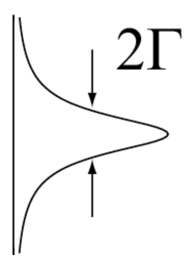
- Quantum fluctuation: "level broadening" Γ

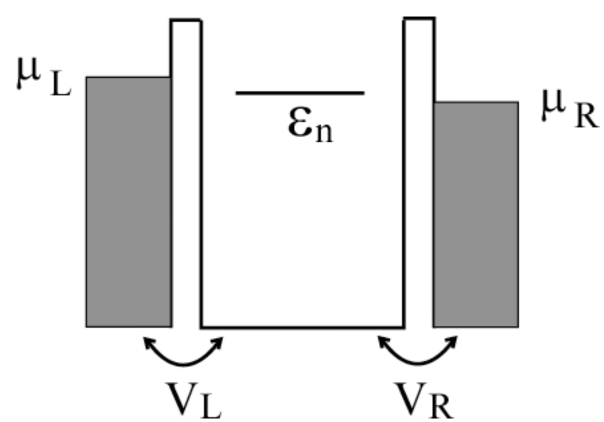
(due to finite lifetime by tunnel coupling to the leads)

$$\frac{1}{\tau} = \sum_{\alpha=L,R;k} \frac{2\pi}{\hbar} \left|\langle \alpha, k | H_T | d_n \rangle\right|^2 \delta(\varepsilon_k - \varepsilon_n)$$

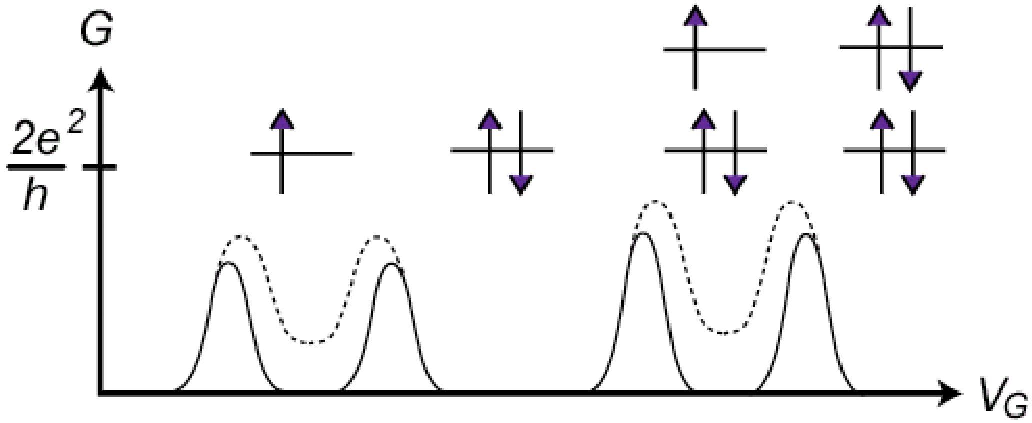
$$= \frac{2\pi}{\hbar} \nu \left(|V_L|^2 + |V_R|^2 \right)$$

$$\Gamma = \frac{1}{2}\frac{\hbar}{\tau} = \pi \nu \left(|V_L|^2 + |V_R|^2 \right)$$





2. Kondo effect in quantum dots with S=1/2



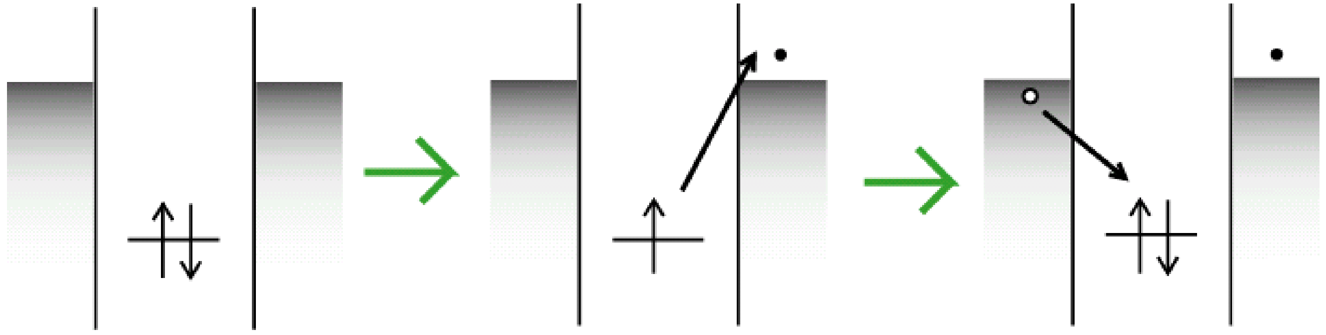
In Coulomb blockade region,

- The number of electrons, N, is fixed.
- Higher-order tunnel processes, "cotunneling current," are dominant.
- Kondo effect enhances the cotunneling current.

odd N: $S=1/2$ (Kondo), even N: $S=0$ (no Kondo)

Higher-order tunneling processes “Cotunneling”

- 2nd order tunnel process through virtual state

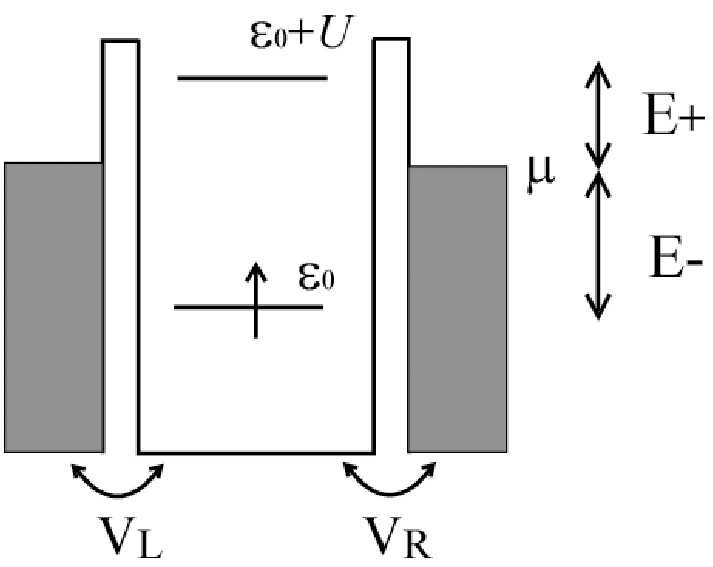


$$V_{\rm R}^{*}\frac{1}{\varepsilon - H_0}V_{\rm L} \approx -\frac{V_{\rm R}^{*}V_{\rm L}}{E^{-}}.$$

Cotunneling: more than one electron participates.

Impurity Anderson model (single level in quantum dot)

$$
\begin{aligned}
H &= H_{\text{leads}} + H_{\text{dot}} + H_{\text{T}}, \\
H_{\text{dot}} &= \sum_{\sigma} \varepsilon_0 d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow, \\
H_{\text{leads}} &= \sum_{\alpha=L,R} \sum_{k\sigma} \varepsilon_k c_{\alpha,k\sigma}^\dagger c_{\alpha,k\sigma}, \\
H_{\text{T}} &= \sum_{\alpha=L,R} \sum_{k\sigma} (V_\alpha c_{\alpha,k\sigma}^\dagger d_\sigma + \text{h.c.}).
\end{aligned}
$$

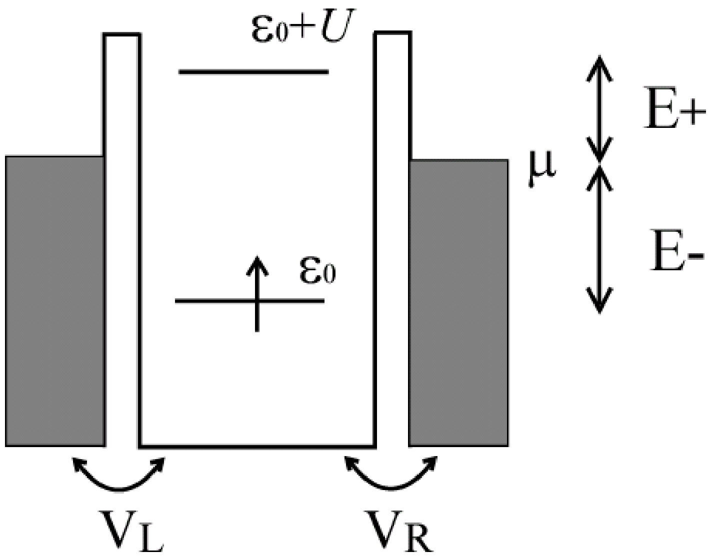


- Coulomb blockade region

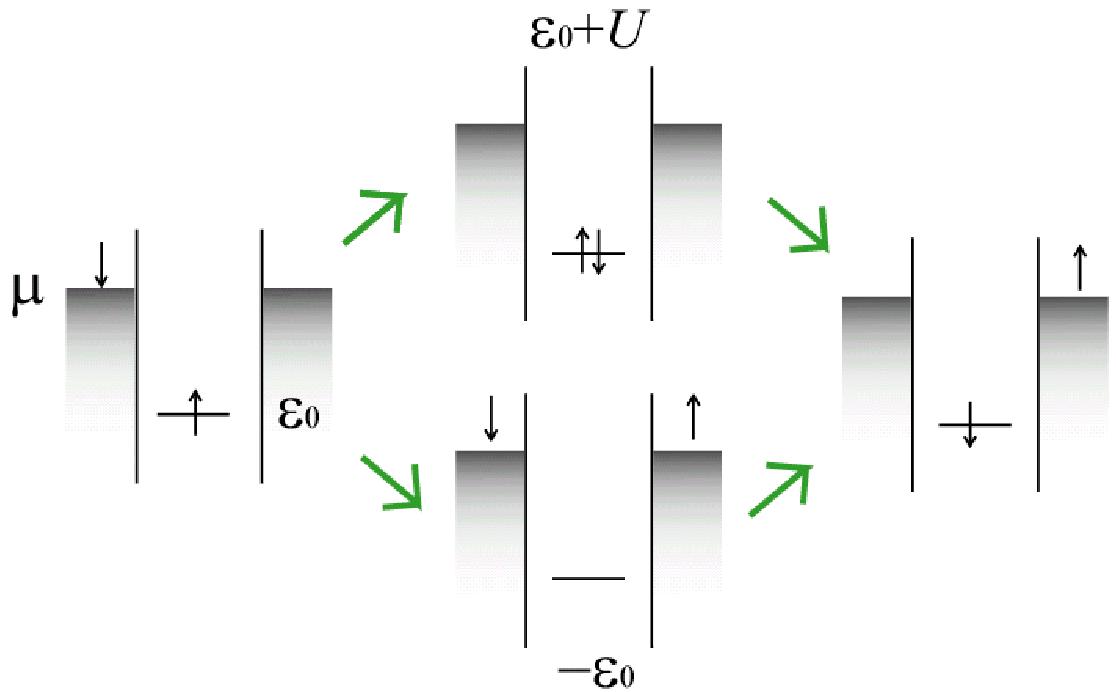
$$E^+, E^- >> k_B T, \Gamma$$

- Addition and extraction energies

$$\begin{cases} E^+ = \mu_2 - \mu = \varepsilon_0 + U - \mu \\ E^- = \mu - \mu_1 = \mu - \varepsilon_0 \end{cases}$$



• S=1/2 in the dot: Spin-flip by cotunneling



$$V_R^* \left[\frac{-1}{\varepsilon - (\varepsilon_0 + U)} + \frac{1}{\varepsilon - \varepsilon_0} \right] V_L = V_R^* \left(\frac{1}{E^+} + \frac{1}{E^-} \right) V_L \equiv \frac{V_R^* V_L}{E_c}$$

at $\varepsilon = \mu$.

Without freedom of charge, with freedom of spin

Effective Hamiltonian for quantum dot with S=1/2

- Second order in H_T (Schrieffer-Wolff transformation)

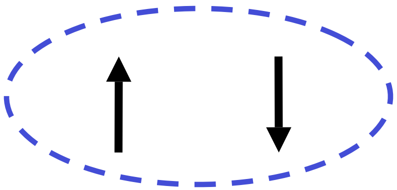
$$\begin{aligned} H &= \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \sum_{kk'} \left[\hat{S}_+ c^\dagger_{k'\downarrow} c_{k\uparrow} + \hat{S}_- c^\dagger_{k'\uparrow} c_{k\downarrow} + \hat{S}_z (c^\dagger_{k'\uparrow} c_{k\uparrow} - c^\dagger_{k'\downarrow} c_{k\downarrow}) \right] \\ &= \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + 2J \sum_{kk'} \mathbf{S} \cdot (\mathbf{s})_{k',k} \end{aligned}$$

with $J = V^2/E_c$ $(1/E_c = 1/E^+ + 1/E^-)$.

"Kondo Hamiltonian": Anti-ferromagnetic coupling between dot spin, $\boldsymbol{S}$, and spins in Fermi sea, $(\boldsymbol{s})_{k',k}$.

Ground state with antiferromagnetic coupling

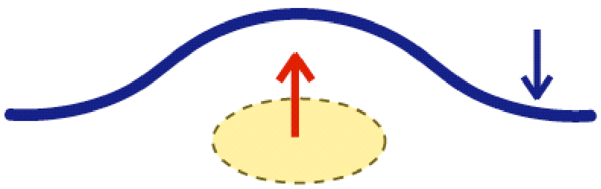
- Two interacting spins:



$$|\mathrm{Grd}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2\right)$$

Spin-singlet state

- One spin and Fermi sea:

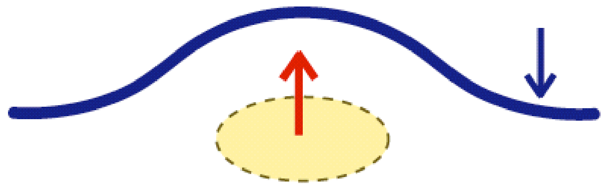


$$|\mathrm{Grd}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{\mathrm{dot}} |\Downarrow\rangle - |\downarrow\rangle_{\mathrm{dot}} |\Uparrow\rangle\right)$$

Kondo singlet state
(Many-body state)

Conduction electrons coherently couple with localized spin. The spin is completely screened.

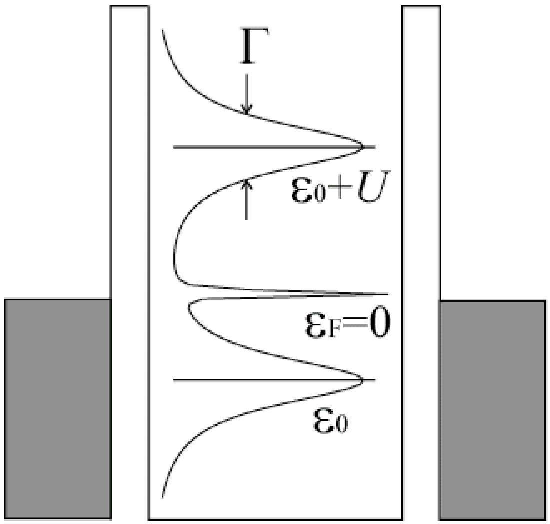
- Kondo temperature T_K: binding energy of the Kondo singlet state



- $T \gg T_K$: Spin $S=1/2$ is not screened out.
- $T \ll T_K$: Kondo singlet state is formed; Spin is screened. Resonant tunneling through the singlet state.

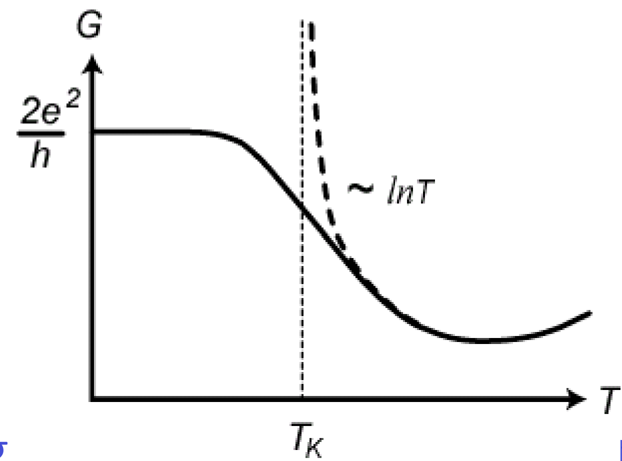
$$G = \frac{2e^2}{h} \frac{4\Gamma_L \Gamma_R}{(\Gamma_L + \Gamma_R)^2}$$

Asymmetric factor



Transmission probability=1 (unitary limit) in symmetric case

- Conductance through quantum dot



Strong coupling (Kondo singlet state; Fermi liquid)

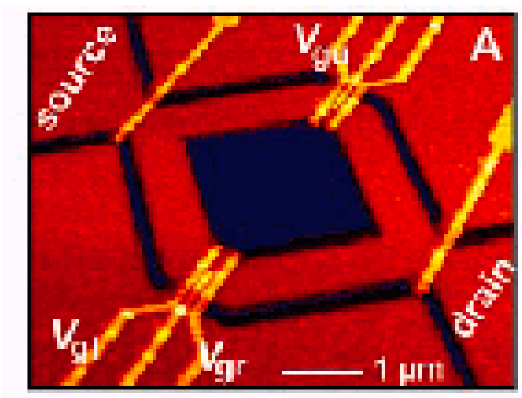
Weak coupling (perturbation; logarithmic *T* dependence)

In quantum dots, Kondo resonance increases the conductance: “Conductance minimum”

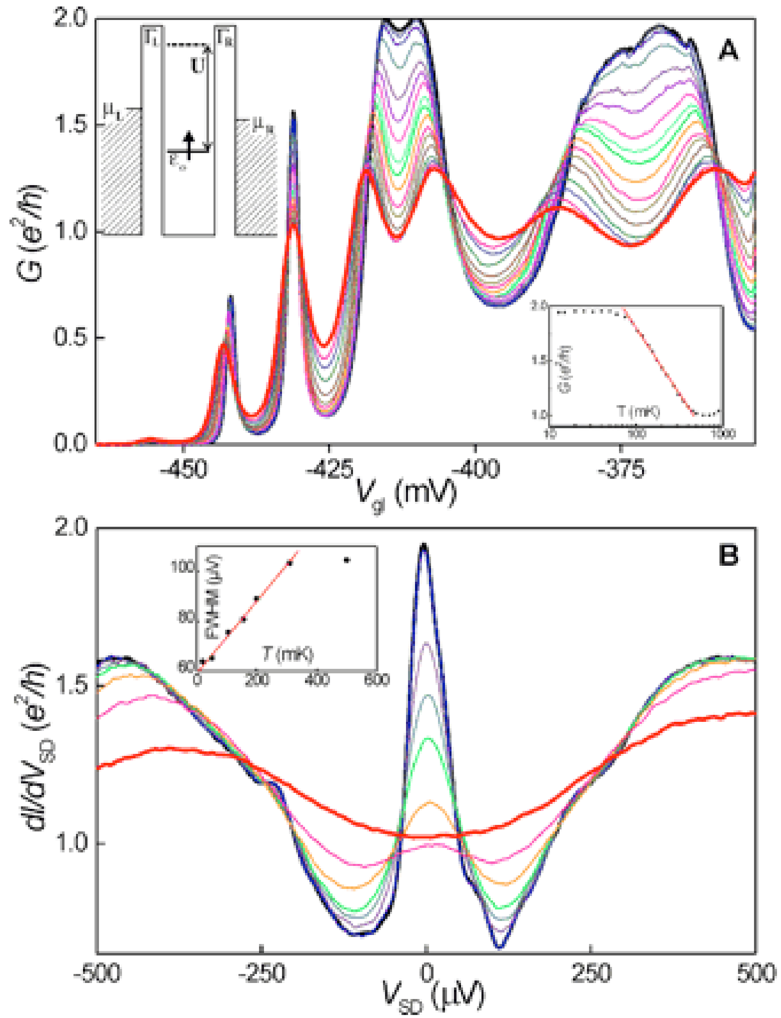
In metals with magnetic impurities, scattering is enhanced resonantly: “Resistivity minimum”

Observation of Kondo effect

W. van der Wiel *et al*., Science **289**, 2105 (2000).

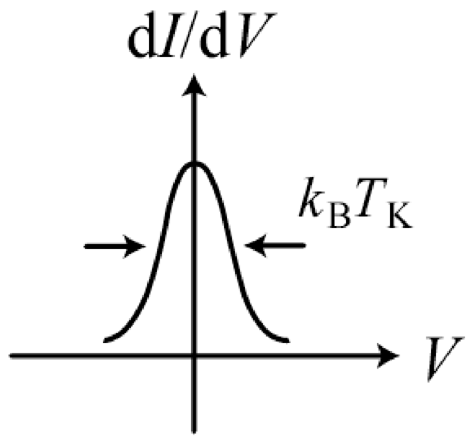


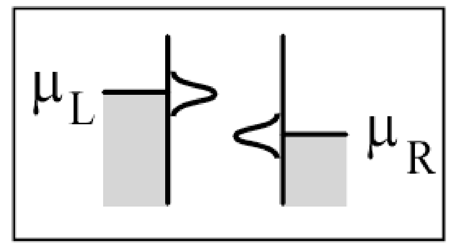
One of the arms is pinched off.



- Finite bias V :

Zero-bias peak of differential conductance





“Direct observation” of resonant peak although non-equilibrium transport has not been understood completely (many-body effect + decoherence).

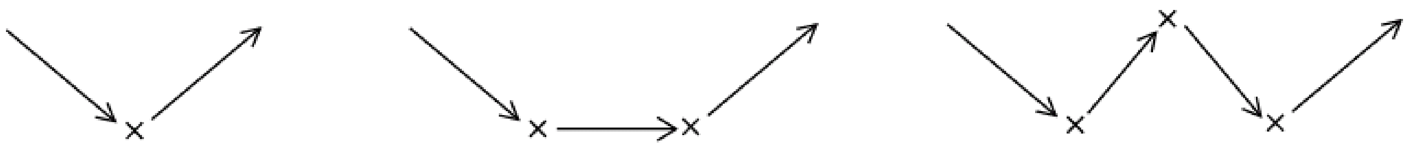
Theory of Kondo effect

(I) Weak coupling regime (T>>T_K):
Scattering problem by dot spin (S=1/2)

$$H = H_0 + V \qquad H_0 = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}, \quad V = 2J \sum_{kk'} \mathbf{S} \cdot (\mathbf{s})_{k',k}.$$

Perturbation with respect to V

$$\hat{T} = V + V\frac{1}{\varepsilon - H_0 + \mathrm{i}\delta}V + V\frac{1}{\varepsilon - H_0 + \mathrm{i}\delta}V\frac{1}{\varepsilon - H_0 + \mathrm{i}\delta}V + \cdots.$$



Born approximation in presence of Fermi sea.

T-matrix (ε: energy of incident electron)

$$\hat{T} = H_{\mathrm{T}} + H_{\mathrm{T}} \frac{1}{\varepsilon - H_0 + \mathrm{i}\delta} H_{\mathrm{T}} + H_{\mathrm{T}} \frac{1}{\varepsilon - H_0 + \mathrm{i}\delta} H_{\mathrm{T}} \frac{1}{\varepsilon - H_0 + \mathrm{i}\delta} H_{\mathrm{T}} + \cdots .$$

Transition probability

$$\frac{2\pi}{\hbar} \left| \langle \mathrm{init} | \hat{T} | \mathrm{fin} \rangle \right|^2 \delta(\varepsilon_{\mathrm{fin}} - \varepsilon_{\mathrm{init}}).$$

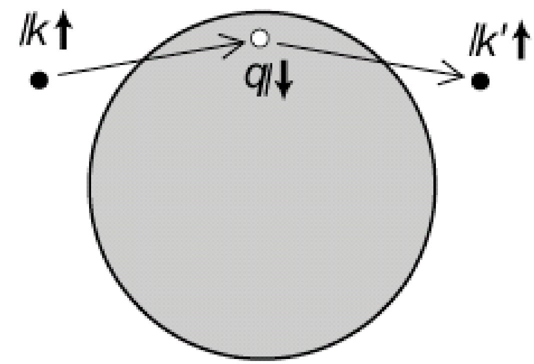
Current from lead L to R

$$\Gamma_{L\to R} = 2 \sum_k \sum_{k'} \frac{2\pi}{\hbar} \left| \langle Rk' | \hat{T} | Lk \rangle \right|^2 \delta(\varepsilon_{Rk'} - \varepsilon_{Lk}) \times f(\varepsilon_{Lk} - \mu_L) \left[1 - f(\varepsilon_{Rk'} - \mu_R) \right] .$$

$$I = e(\Gamma_{L\to R} - \Gamma_{R\to L}) \quad \text{with} \quad eV = \mu_L - \mu_R$$

Second Born processes

- Logarithmic divergence by the virtual process with spin flip (J. Kondo, 1964)



$$\langle \uparrow; k' \uparrow | \hat{T} | \uparrow; k \uparrow \rangle = \begin{cases} -\nu J^2 \ln |\varepsilon| / D & \text{for } |\varepsilon| >> k_B T \\ -\nu J^2 \ln k_B T / D & \text{for } |\varepsilon| << k_B T \end{cases}$$

(D: bandwidth of conduction electrons in Fermi sea)

(i) Precursor to the formation of Kondo singlet.
(ii) Contribution from high energy; "scale invariance"

- Leading order logarithmic terms (Abrikosov)

$$\langle \uparrow ; k' \uparrow | \hat{T} | \uparrow ; k \uparrow \rangle = \frac{J/2}{1 + 2\nu J \ln k_B T / D} \quad \text{for } |\varepsilon| << k_B T$$

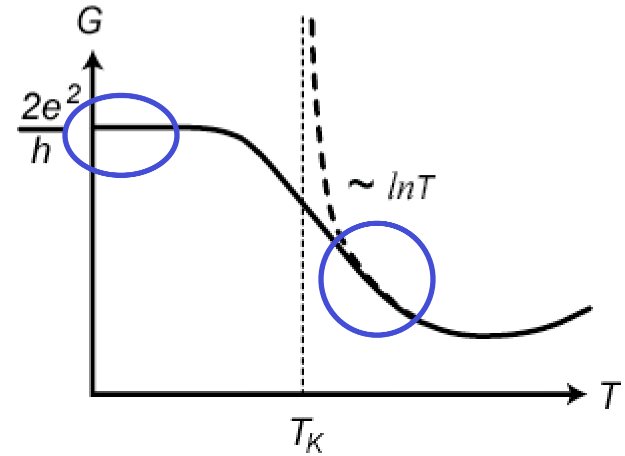
Diverges at Kondo temperature : $T_K = D \exp(-1/2\nu J)$

$$G = \frac{2e^2}{h} \frac{4\Gamma_L \Gamma_R}{(\Gamma_L + \Gamma_R)^2} \frac{3\pi^2}{16} \frac{1}{[\ln(T/T_K)]^2}$$

(II) Strong coupling regime ($T<<T_K$):

Fermi liquid theory with a resonance

$$G = \frac{2e^2}{h} \frac{4\Gamma_L \Gamma_R}{(\Gamma_L + \Gamma_R)^2} \left[1 - \pi^2 (T/T_K)^2\right]$$



Conjecture from (I) and (II); with a universal function F

$$G = \frac{2e^2}{h} \frac{4\Gamma_L \Gamma_R}{(\Gamma_L + \Gamma_R)^2} F(T / T_K)$$

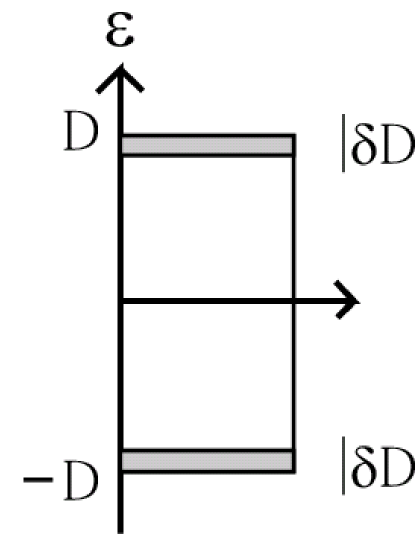
- Only one relevant energy scale, T_K
- Universal function of max(T, B)/T_K
- Kondo temperature T_K depends on microscopic parameters; J (ε_0, U ,$V_{L,R}$, ν), D.

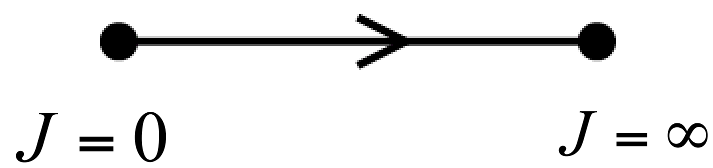
(III) Scaling theory

- We are interested in transport of energy scale T.
- High energy scale is truncated by the renormalization of J.

Poor man's scaling (Anderson)

- Based on 2^{nd} order perturbation in J
- Bandwidth D is changed.
- Exchange coupling J is renormalized not to change the low energy physics.
- J increases with decreasing D. (The perturbation becomes worse).
- Scaling equation: J diverges at $D=T_K$





Numerical renormalization group (NRG, Wilson)

- "Exact" renormalization procedure (numerical)
- Most reliable method to calculate the Kondo effect

3. Kondo effect in multi-level quantum dots: experimental results

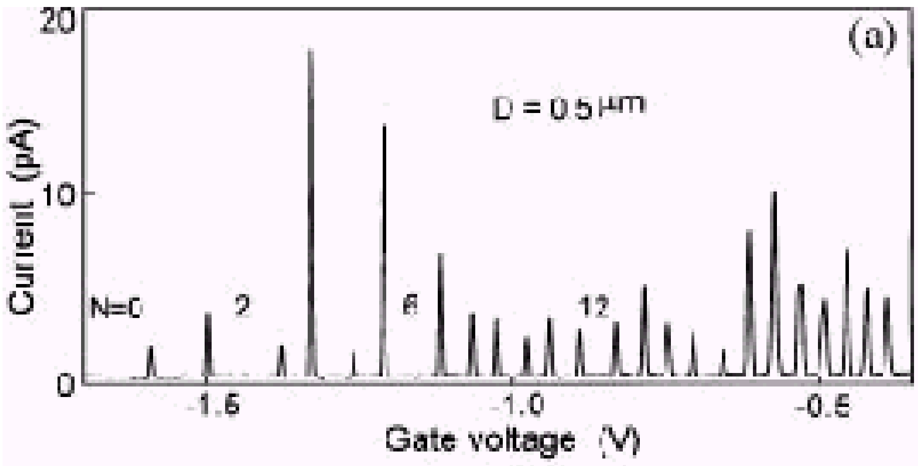
(I) SU(4) Kondo effect with S=1/2 at orbital degeneracy

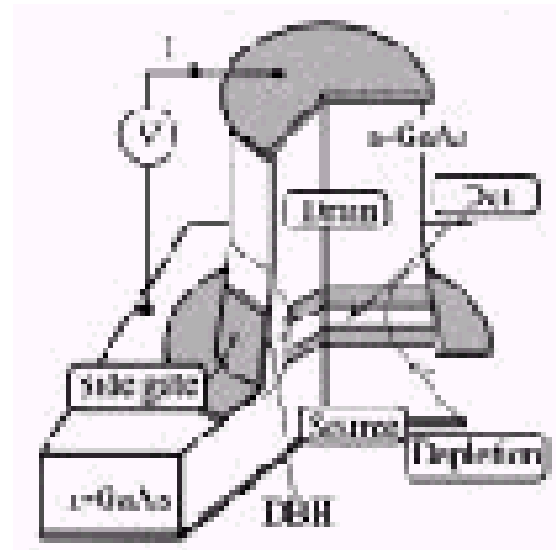
Sasaki *et al*., PRL (2004) [Tarucha group]

(II) Kondo effect at singlet-triplet degeneracy with an even number of electrons

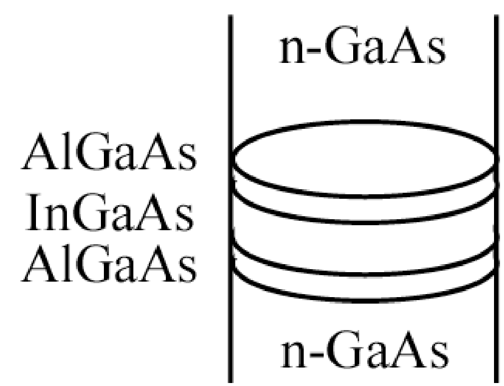
Sasaki *et al*., Nature (2000) [Tarucha and Kouwenhoven groups]

Vertical quantum dots: Tarucha *et al*. (1996)

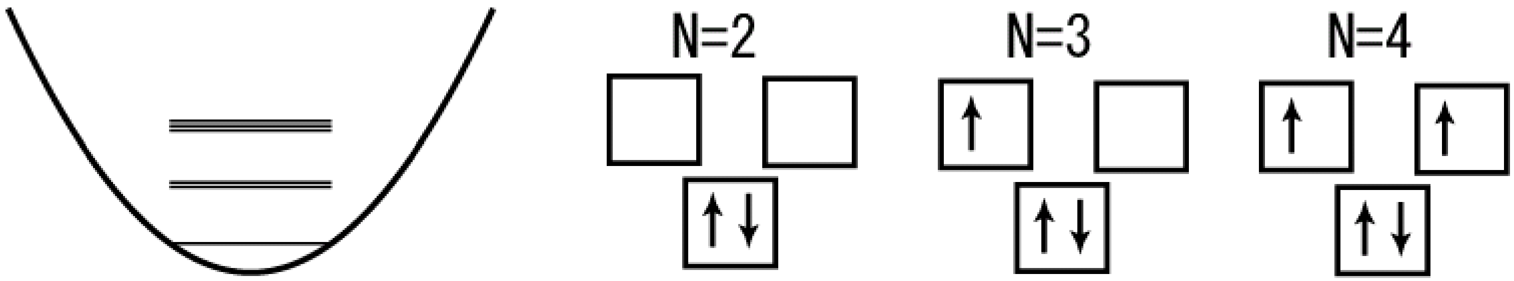




- Quantum dots of disk shape
- N=0, 1, 2, 3, …

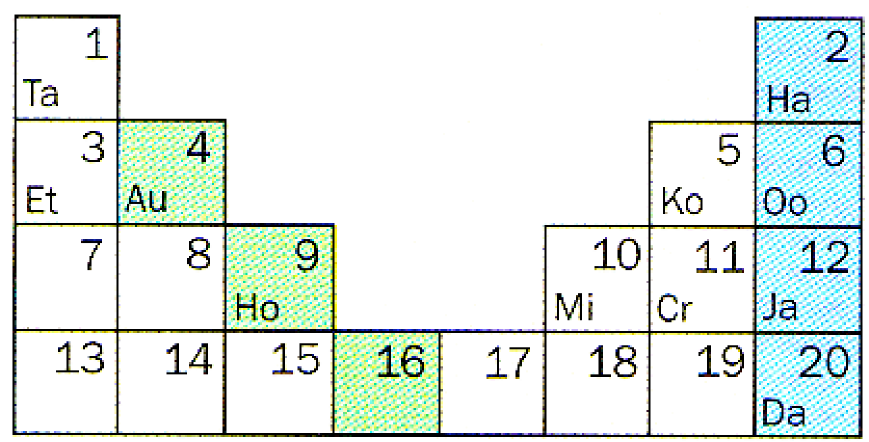


2D harmonic potential



- Shell structure of one-electron levels
- Parallel spins at degenerate levels (*N*=4) due to exchange interaction (Hund's rule).
- Artificial atoms

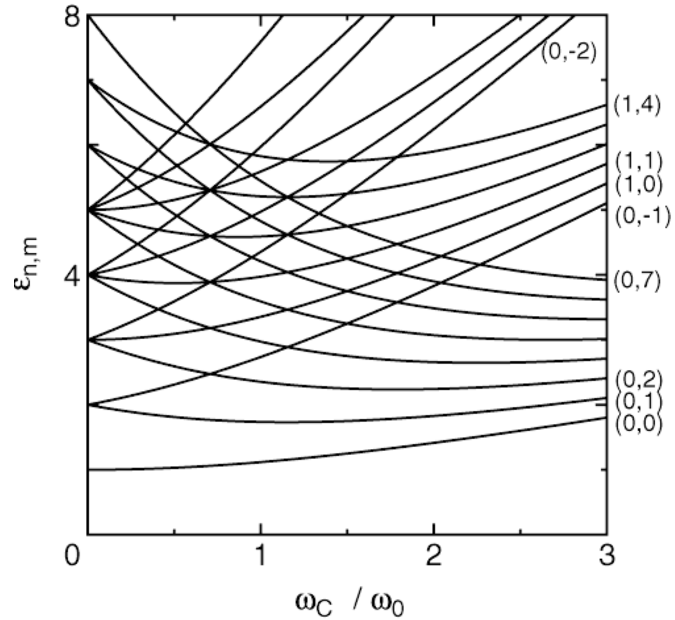
"Periodic table"

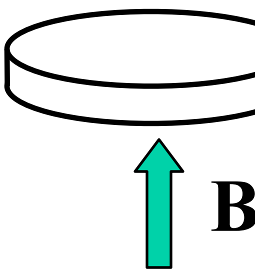


Kouwenhoven and Marcus, Physics World (June, 1998).

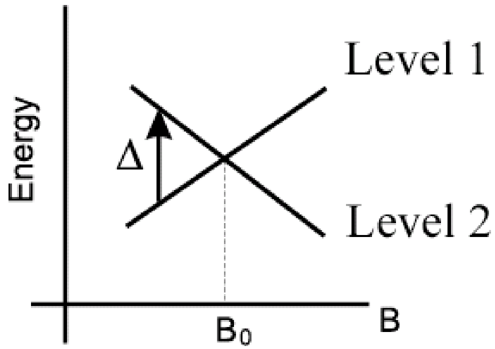
Tunable energy levels by magnetic field

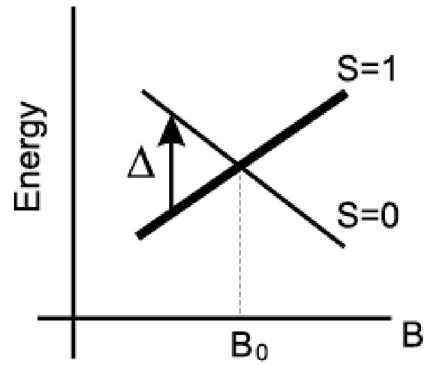
Darwin-Fock diagram:





- Odd *N*: Level spacing
- Even *N*: *S*=1 (triplet) to *S*=0 (singlet) transition.

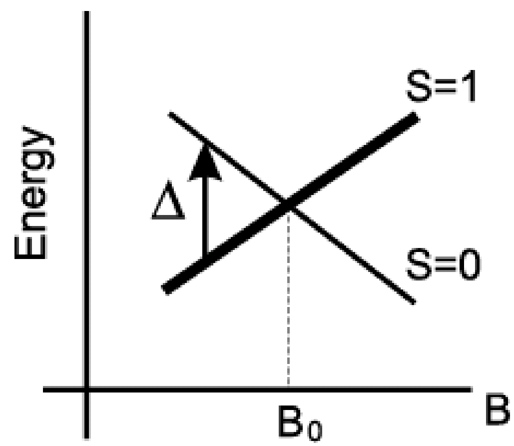




3.1. Kondo effect with an even number of electrons

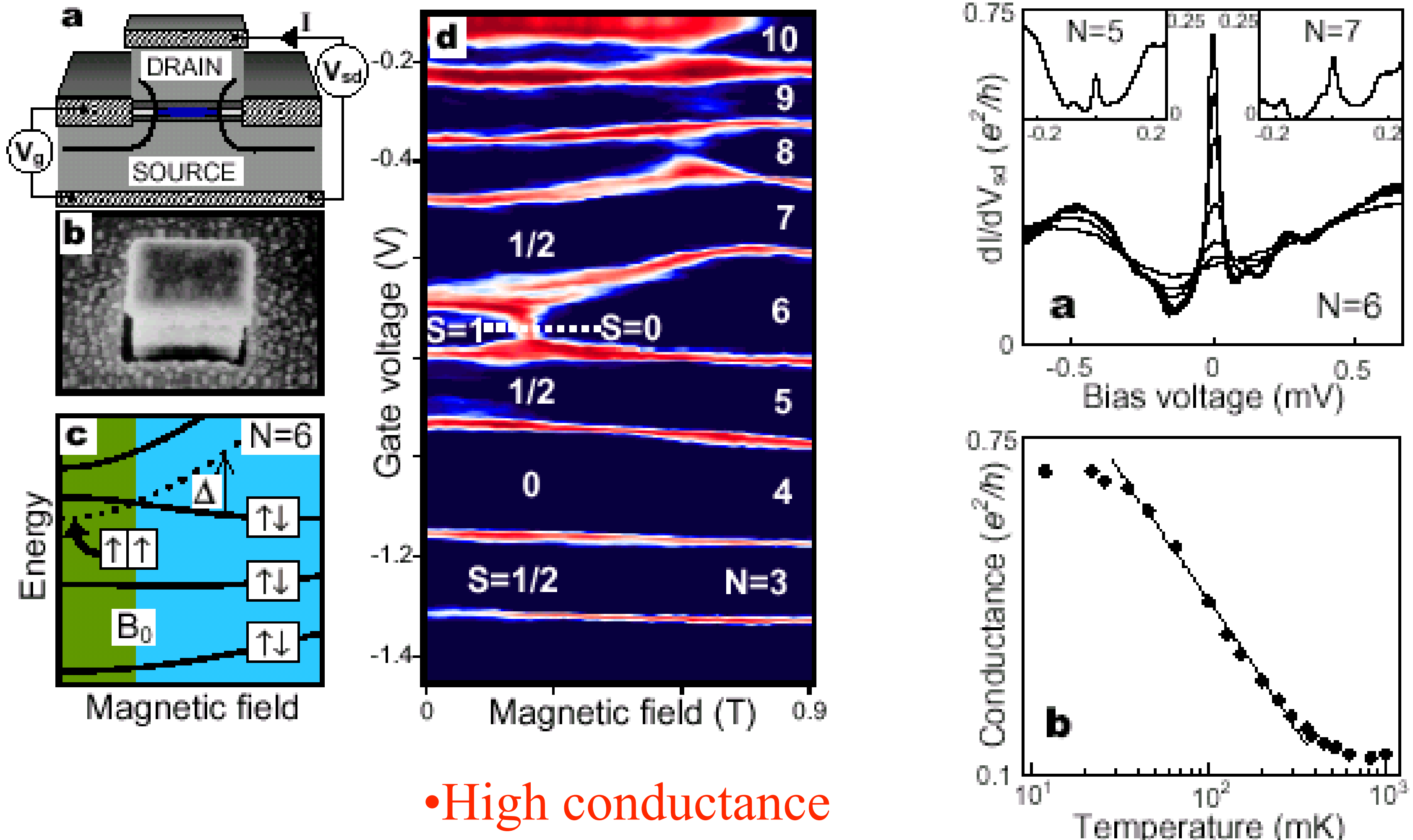
Sasaki *et al.*, Nature **405**, 764 (2000).

- Energy difference between spin-singlet and triplet is tuned by magnetic field.



- Zeeman effect is negligible (g^*=0.4, B=0.2T). Zeeman energy=40mK << T_K=350 mK.

Enhanced Kondo effect at singlet-triplet degeneracy



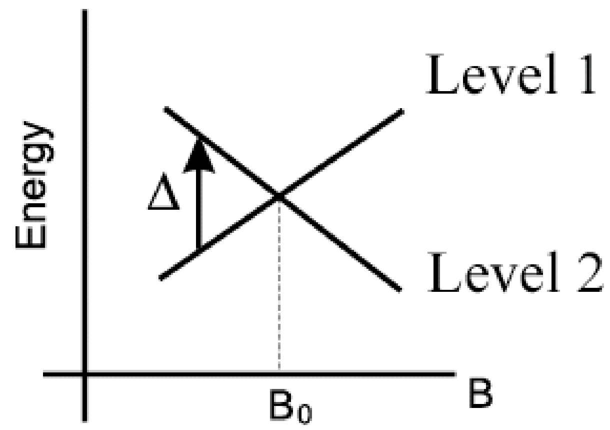
•High conductance

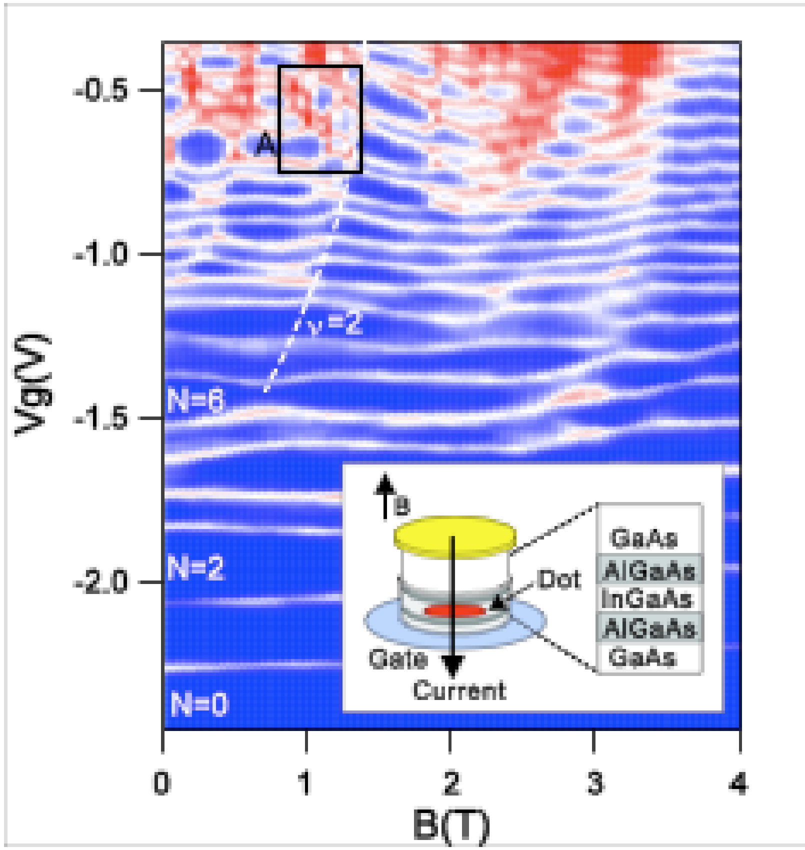
•Low conductance

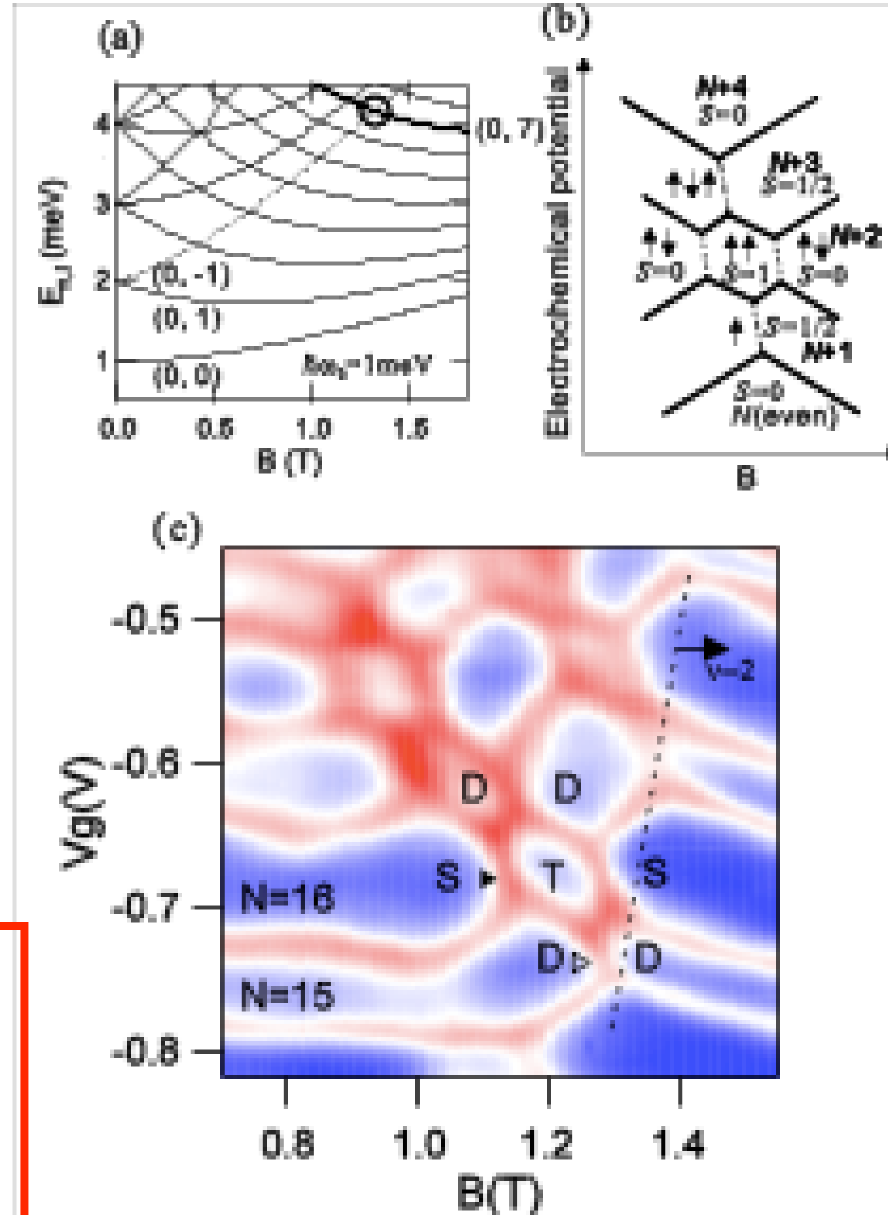
3.2. Kondo effect with S=1/2 and orbital degeneracy

Sasaki *et al*., PRL **93**, 17205 (2004).

- Energy level separation is tuned by magnetic field.
- A large Kondo effect around Δ=0







Orbital symmetry (angular momentum) is conserved in tunneling processes;
Two channels in leads

Four-fold degeneracy enhances the Kondo effect in both cases.

- Singlet-triplet degeneracy

$$|S=0, S_z=0\rangle,$$
$$|S=1, S_z=1\rangle, |1,0\rangle, |1,-1\rangle$$

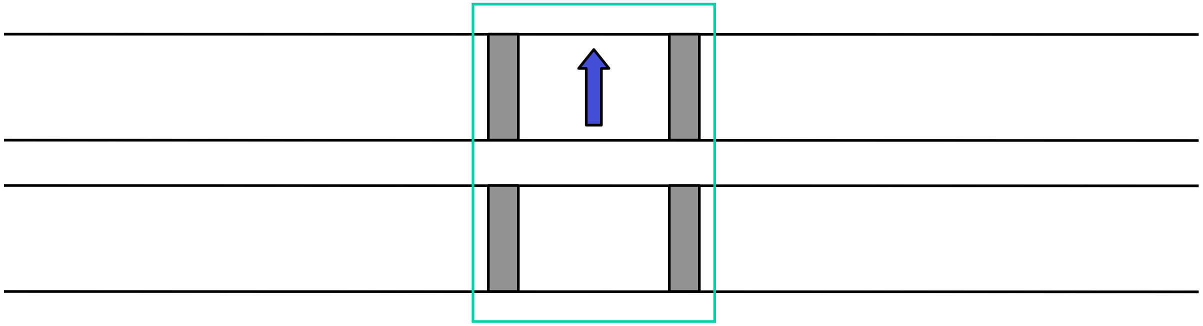
Theory: M.Eto and Yu.V.Nazarov, PRL (2000); M. Pustilnik and L. I. Glazman, PRL (2000).

- S=1/2 and orbital degeneracy: SU(4) symmetry

$$|\uparrow, \text{orbital } 1\rangle, |\downarrow, \text{orbital } 1\rangle, |\uparrow, \text{orbital } 2\rangle, |\downarrow, \text{orbital } 2\rangle$$

Recent experiment using double quantum dots

A. Huebel, J. Weis and K.v.Klitzing (Stuttgart)



One electron in double QDs
(large interdot Coulomb interaction)

- SU(4) Kondo effect:

$$\left|\uparrow,\mathrm{dot}\ 1\right\rangle,\left|\downarrow,\mathrm{dot}\ 1\right\rangle,\left|\uparrow,\mathrm{dot}\ 2\right\rangle,\left|\downarrow,\mathrm{dot}\ 2\right\rangle$$

4. Theory of SU(4) Kondo effect in quantum dots

4.1. SU(4) Kondo effect

- One electron (S=1/2), two degenerate orbitals
- Previous work for magnetic impurity with f electrons (total angular momentum j)

  Coqblin-Schrieffer model of SU(N_d) symmetry:

  The total degeneracy factor $N_d=2j+1$ increases T_K.

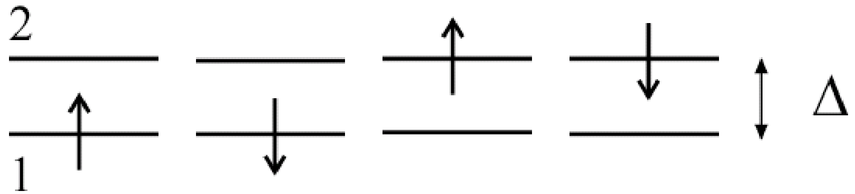
$$k_B T_K = D_0 e^{-1/N_d \nu J}$$

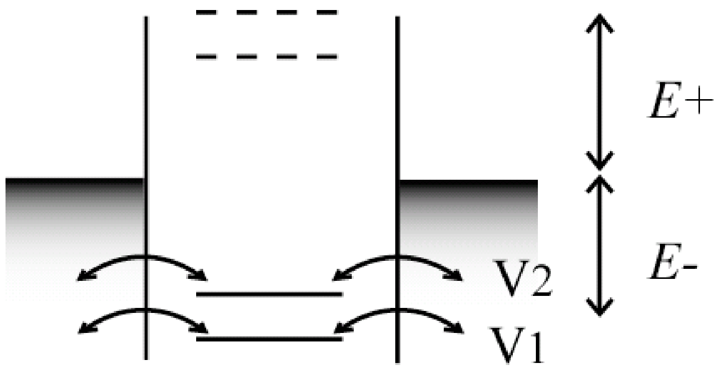
- In quantum dots, Δ is tunable; lower symmetry?

4.2. Model

- A quantum dot with an electron (S=1/2) and two orbitals (*i*=1,2).
- Energy-level separation

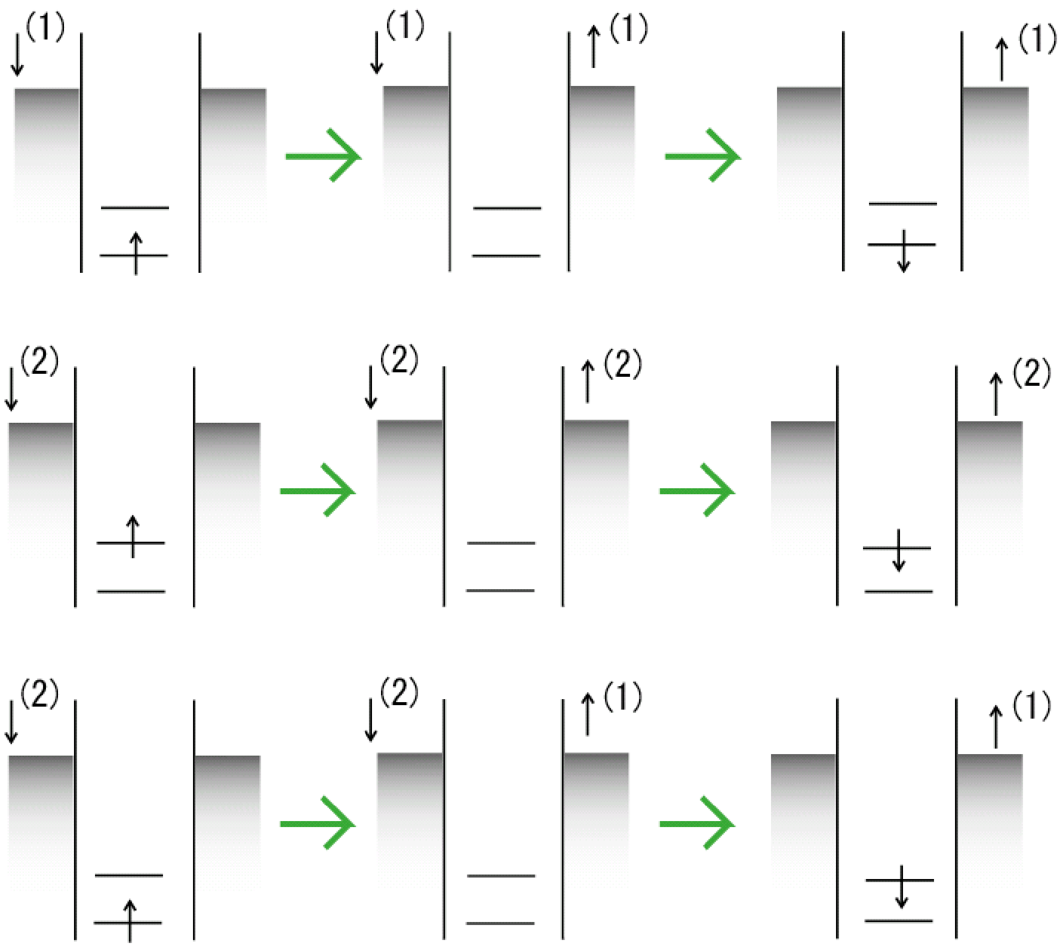
$$\Delta = \varepsilon_2 - \varepsilon_1$$





(Two channels in the leads.)

Exchange couplings



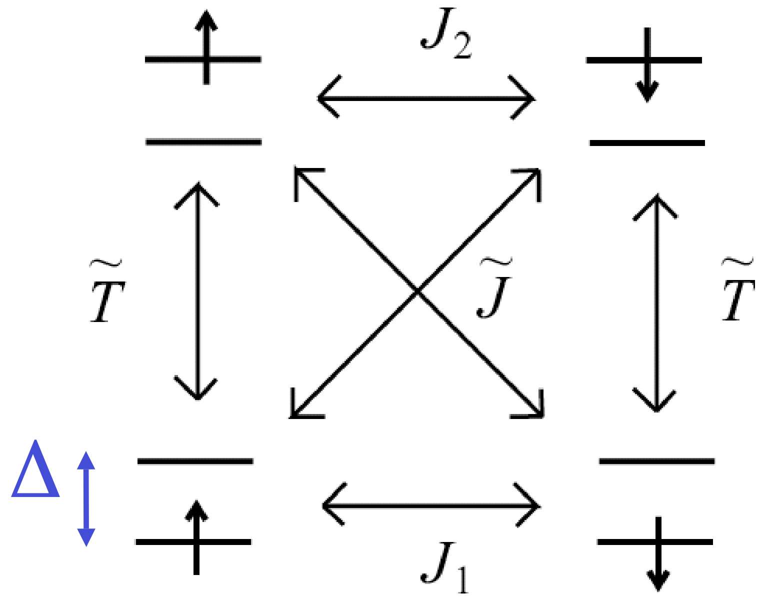
$$J_1 = V_1^2 / \widetilde{E}_C$$

$$J_2 = V_2^2 / \widetilde{E}_C$$

$$\widetilde{J} = \widetilde{T} = V_1 V_2 / \widetilde{E}_C$$

(with and without spin flip)

There are four exchange couplings.



$$J_1 = V_1^2 / \tilde{E}_C,$$
$$J_2 = V_2^2 / \tilde{E}_C,$$
$$\tilde{J} = \tilde{T} = V_1 V_2 / \tilde{E}_C$$
$$\left(1/\tilde{E}_C = 1/E^+ + 1/E^-\right)$$

Symmetric case of $V_1 = V_2$:

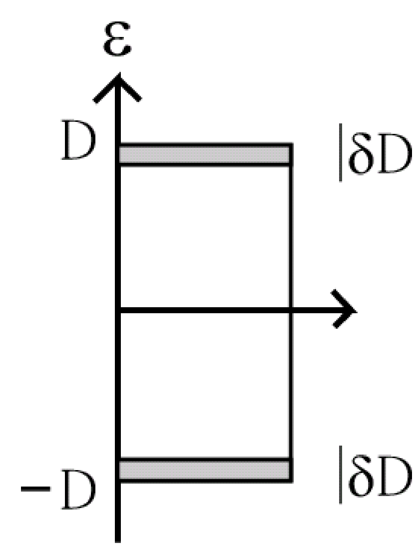
$$J_1 = J_2 = \tilde{J} = T \equiv J. \quad \text{When } \Delta = 0, \text{SU(4) symmetry}$$

(*) Single orbital, spin 1/2: SU(2) symmetry

4.3. Symmetric tunneling case ($V_1=V_2$)

Poor man's scaling method (Anderson)

- Based on perturbation with respect to J
- Bandwidth D (energy scale) is changed (*).
- Exchange coupling J is renormalized not to change the low energy physics.
- With decreasing D, J increases. (The perturbation becomes worse.)
- Scaling equation: J diverges at $D=T_K$



(*) Initially, $D_0 = \sqrt{E_+ E_-}$

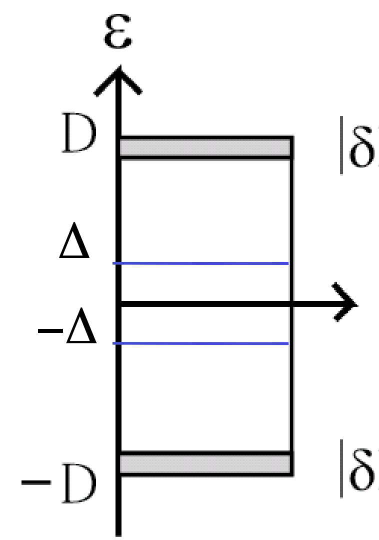
Scaling equations for D-D Kondo effect

- When $D >> |\Delta|$, J develops rapidly with decreasing D, due to the four-fold degeneracy [SU(4) Kondo effect].

$$dJ / d \ln D = -4\nu J^2$$

- When $D << |\Delta|$, the evolution of J is slower since the higher orbital is irrelevant [SU(2) Kondo].

$$dJ / d \ln D = -2\nu J^2$$



- At $D \sim |\Delta|$, the solutions of these equations are connected [crossover from SU(4) to SU(2) Kondo effect].

Kondo temperature as a function of Δ: $T_K(\Delta)$

- When $|\Delta| \ll T_K$, $T_K(\Delta)$ is maximal [SU(4) Kondo]:

$$T_K(0) = D_0 \exp\left[-1/4\nu J\right]$$

- When $|\Delta| \gg D_0$ [SU(2) Kondo],

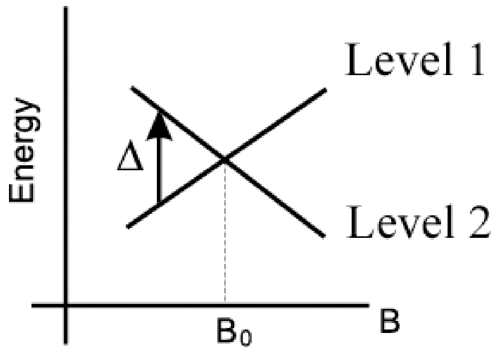
$$T_K(\infty) = D_0 \exp\left[-1/2\nu J\right]$$

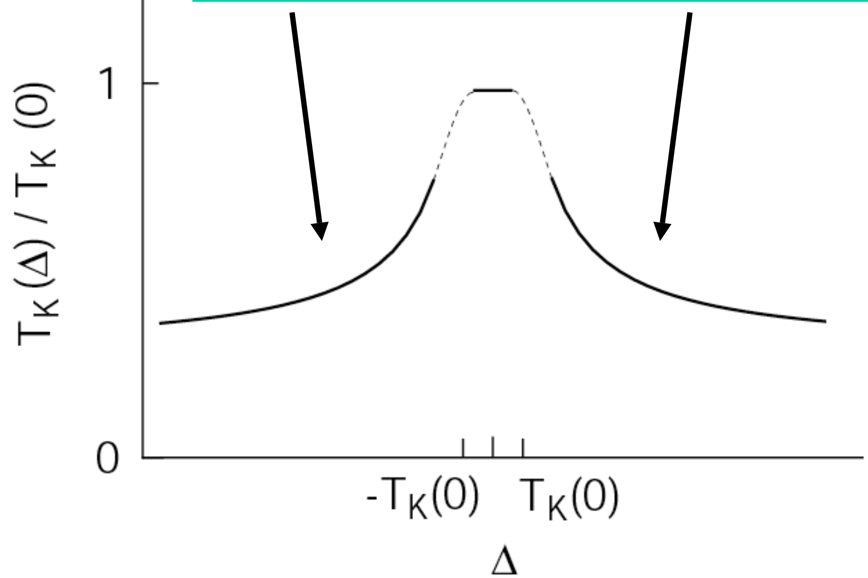
- $T_K(0) \ll |\Delta| \ll D_0$ [crossover from SU(4) to SU(2)],

A pow

$$T_K(\Delta) = T_K(0) \times \left[T_K(0)/|\Delta|\right]^{\gamma}, \quad \gamma = 1$$

$$T_K(\Delta) = T_K(0) \times \left[T_K(0) / |\Delta| \right]^{\gamma},$$
with $\gamma = 1$





- $T_{K,}$ is maximal around $\Delta=0$ [SU(4) Kondo].
- With increasing $|\Delta|$, $T_K(\Delta)$ decreases following a power law [crossover from SU(4) to SU(2)].

cf. K. Yamada, K. Yosida and K. Hanzawa, Prog. Theor. Phys. **71**, 450 (1984).

4.4. General case of $V_1 \neq V_2$

When $D >> |\Delta|$,

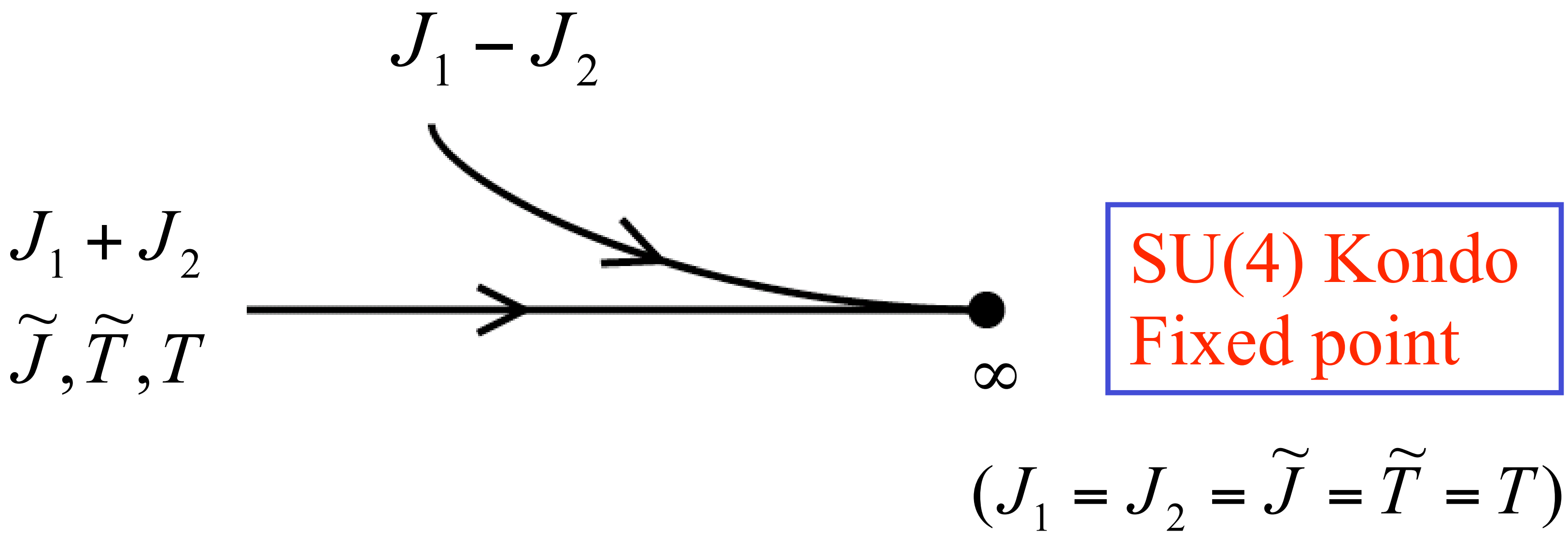
$$\begin{cases} dJ_1 / \nu d \ln D = -2J_1^2 - \tilde{J}(\tilde{J} + \tilde{T}) \\ dJ_2 / \nu d \ln D = -2J_2^2 - \tilde{J}(\tilde{J} + \tilde{T}) \\ d\tilde{J} / \nu d \ln D = -\tilde{J}(J_1 + J_2 + \tilde{T}) - \tilde{T}(J_1 + J_2)/2 \\ d\tilde{T} / \nu d \ln D = -3\tilde{J}(J_1 + J_2)/2 - \tilde{T}T \\ dT / \nu d \ln D = -3\tilde{J}^2 - \tilde{T}^2 \end{cases}$$

When $D << |\Delta|$,

$$dJ_1 / \nu d \ln D = -2J_1^2 \quad (\text{for } \Delta > 0)$$

Fixed point of SU(4) Kondo effect is marginal.
$T_K(\Delta)$ is not a universal function.

Renormalization flow



Non-universal behavior:

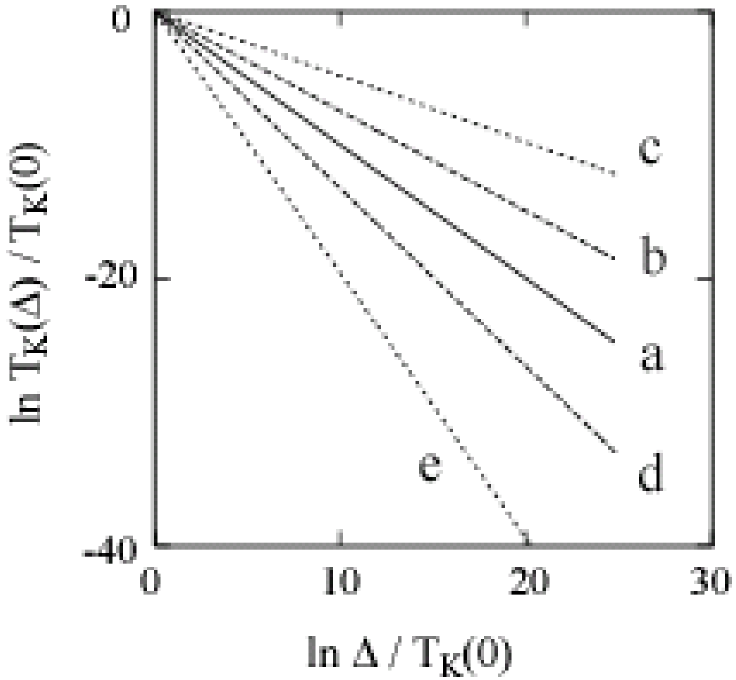
$$T_K(\Delta) = T_K(0) \times \left[T_K(0) / |\Delta| \right]^{\gamma}, \quad \gamma \approx V_2^1 / V_1^2 = \Gamma_2 / \Gamma_1$$

M.Eto, J. Phys. Soc. Jpn. **74**, 95 (2005).

If stable, the fixed point would determine the exponent.

$$T_K(\Delta) = T_K(0) \times \left[T_K(0) / |\Delta|\right]^{\gamma}, \quad \gamma \approx V_2^1 / V_1^2 = \Gamma_2 / \Gamma_1$$

Numerical studies



(a) (broken line): $V_1 = V_2$

(b) $(V_1/V_2)^2 = 3/4$

(c) 1/2

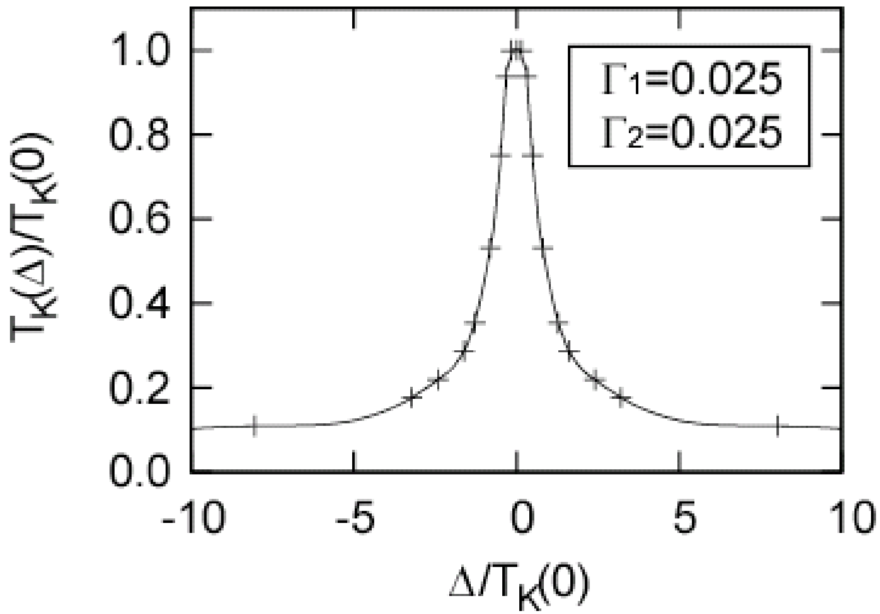
(d) 4/3

(e) 2

A power law holds approximately when $V_1 \sim V_2$.

4.5. NRG studies (with T.Sato and O.Sakai)

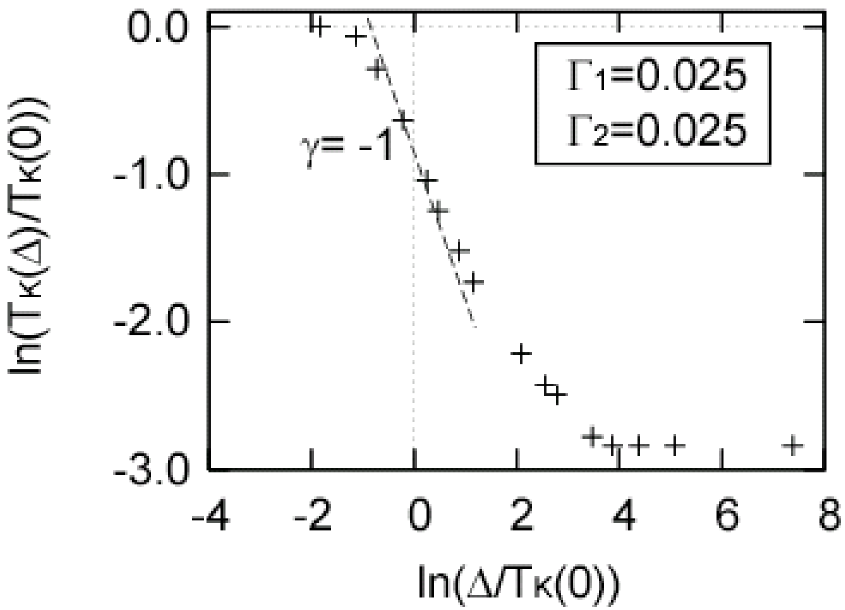
- Kondo temperature as a function of energy difference Δ
- Estimated by magnetic excitation spectrum(*)

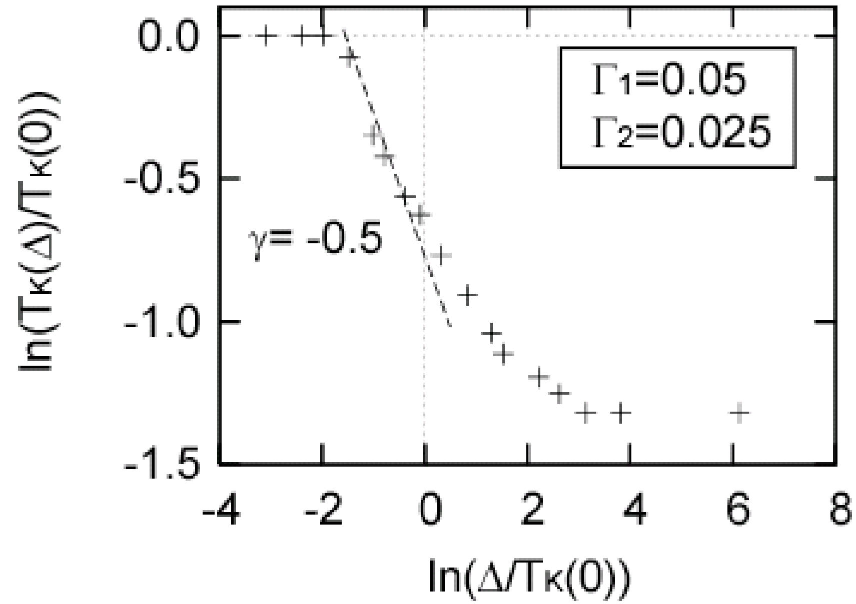


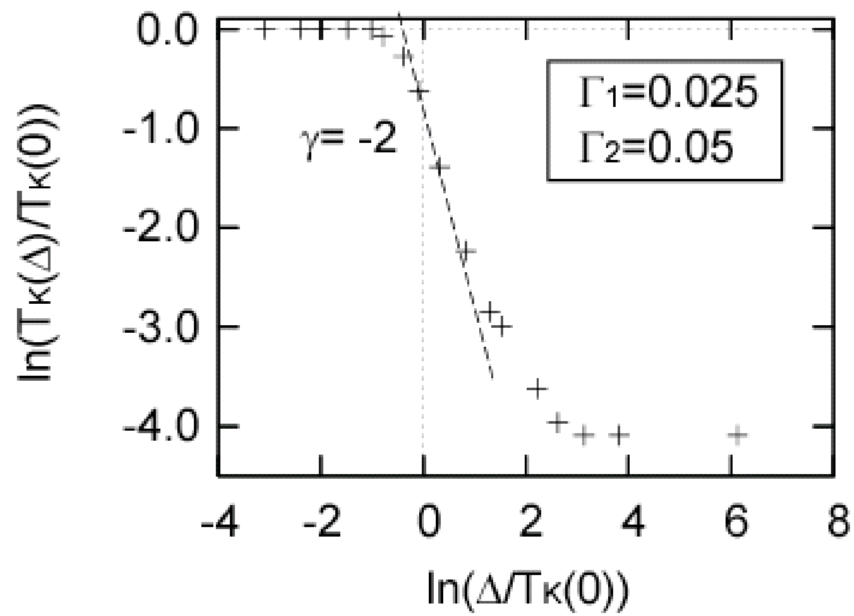
$$(*)\ \chi''(\omega) = \sum_{\mathrm{Gr},n} \left| \langle n | S_{1,z} + S_{2,z} | \mathrm{Gr} \rangle \right|^2 \delta(\omega - E_n + E_{\mathrm{Gr}}),$$

(peak position) ⇔ (characteristic energy of spin fluctuation)

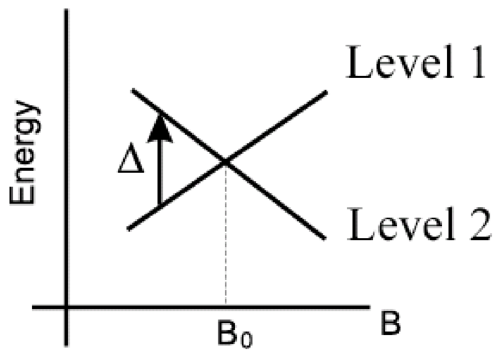
T_K in log-log scale;
power law in a range of Δ

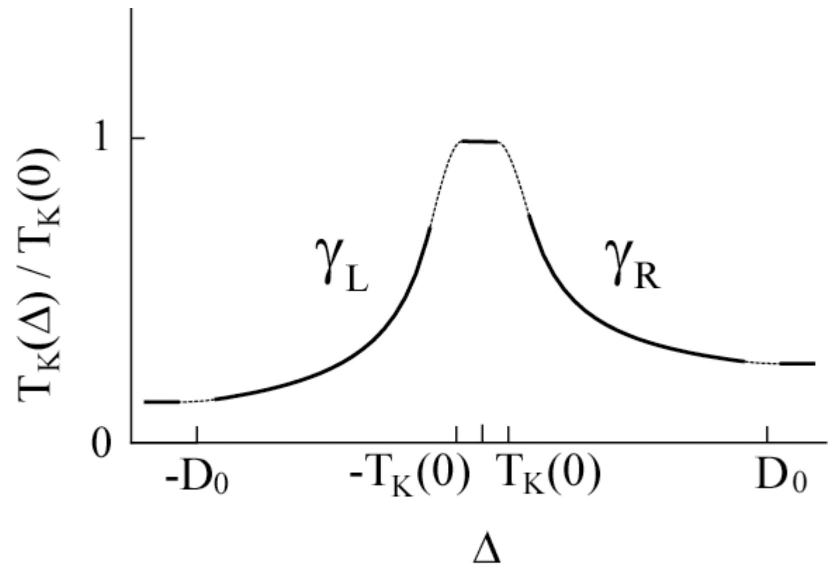






On both sides of level crossing points





$$T_K(\Delta) = T_K(0) \times \left[T_K(0) / |\Delta|\right]^{\gamma}, \qquad \gamma_L \times \gamma_R \approx \frac{\Gamma_2}{\Gamma_1} \times \frac{\Gamma_1}{\Gamma_2} = 1$$

Evidence of marginal fixed point of SU(4) Kondo.

4.6. Conclusions

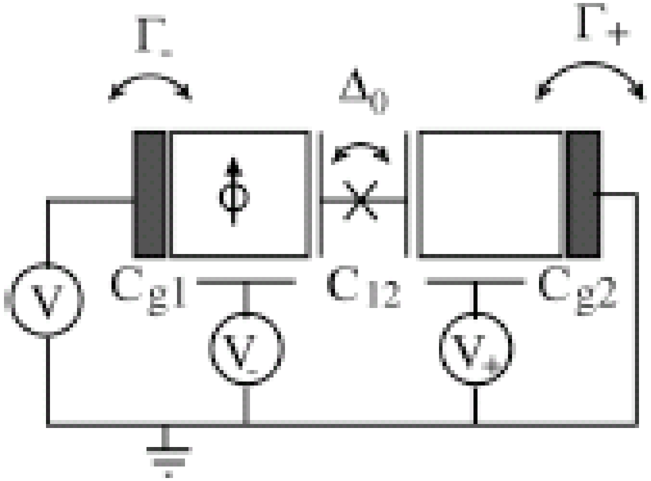
- SU(4) Kondo effect in quantum dots is theoretically examined.
- The Kondo temperature is maximal around a level crossing (energy separation Δ=0) and decreases with increasing $|\Delta|$, obeying a power law [crossover from SU(4) to SU(2) Kondo effect].

$$T_K(\Delta) = T_K(0) \times \left[T_K(0) / |\Delta| \right]^{\gamma}$$

- Generally, $\gamma_L \gamma_R = 1$ where γ_L and γ_R are the exponents on both sides of a level crossing, reflecting marginal fixed point of SU(4) Kondo effect.

Another theoretical work of SU(4) Kondo effect

- Double quantum dots connected in series
  Borda, Zarand, Hofstetter, Halperin, and von Delft, PRL (2003); NRG studies

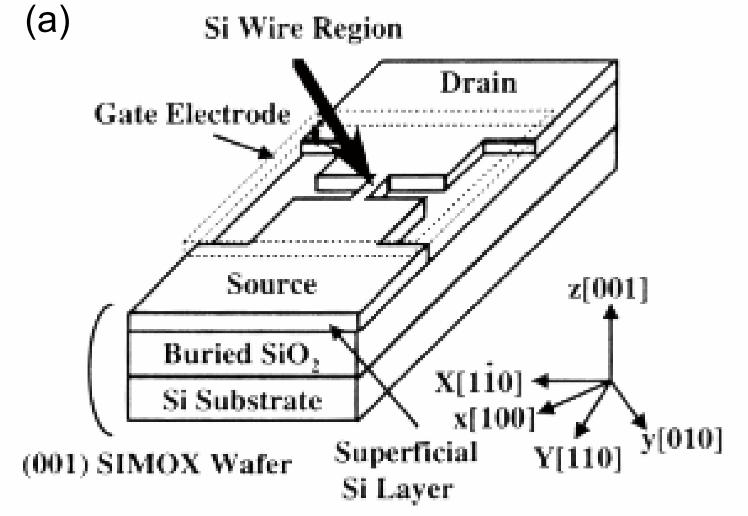


$$\left|\uparrow, \text{dot } L\right\rangle, \left|\downarrow, \text{dot } L\right\rangle,$$
$$\left|\uparrow, \text{dot } R\right\rangle, \left|\downarrow, \text{dot } R\right\rangle$$

- Fermi liquid theory is applicable.
- No evidence of marginal fixed point of SU(4) Kondo.

5. Kondo effect in multi-valley quantum dots

5.1. Introduction: Si quantum dots



Oxidation of Si wires makes an effective quantum dot; small size, unknown shape

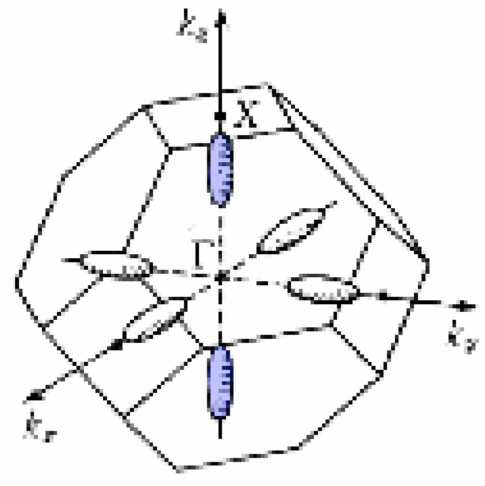
Takahashi *et al*. Electron. Lett. (1995); Horiguchi *et al*. Jpn. J. Appl. Phys (2001); Rokhinson *et al*. PRB (2001).

Properties of Si

- More than one bottom of conduction band (valley): multivalley structure

(1) 6-valley degeneracy in bulk

(2) 2-valley degeneracy in Si-MOS



$\boldsymbol{k} = (0,0,\pm k_0)$, with $k_0 = 0.85 \times 2\pi / a$

($a = 0.543$nm) denoted by $\pm k_z$

cf. single valley at Γ point in GaAs

How is *k*-space degeneracy in real-space confinement of quantum dots?

5.2. Electronic states in Si quantum dots

- Two equivalent valleys are assumed.
- Effective mass approximation (dot size $L >> a$)

$$\psi_{\pm k_z}(\boldsymbol{r}) = F(\boldsymbol{r})\, e^{\pm i k_0 z} u_{\pm k_z}(\boldsymbol{r})$$

- Envelope function $F(\boldsymbol{r})$:

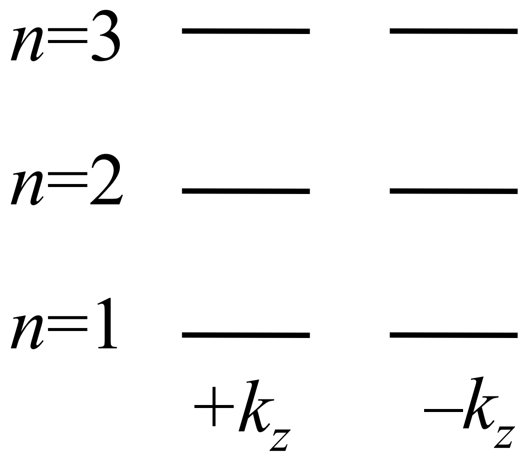
$$\left[-\frac{\hbar^2}{2m_t^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)-\frac{\hbar^2}{2m_l^*}\frac{\partial^2}{\partial z^2}+V(\boldsymbol{r})\right]F(\boldsymbol{r}) = \varepsilon\, F(\boldsymbol{r})$$

$$\left(m_l^* = 0.98\, m_0,\ m_t^* = 0.19\, m_0\right)$$

yields eigenvalues ε_n and eigenfunctions $F_n(\boldsymbol{r})$ (n=1,2,3,…), which are common to both valleys.

(*) linear dispersion for carbon nanotube, graphene.

(I) Single electron levels



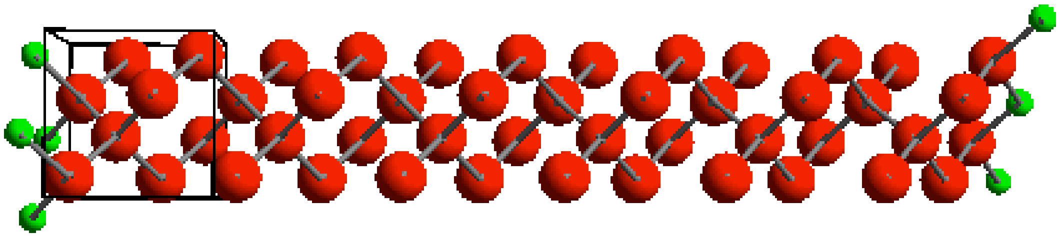
- Two-hold degeneracy due to the equivalent valleys
- Assuming $L>>a$ and smooth confinement (no intervalley scattering)
- Confirmed by empirical tight-binding calculations;

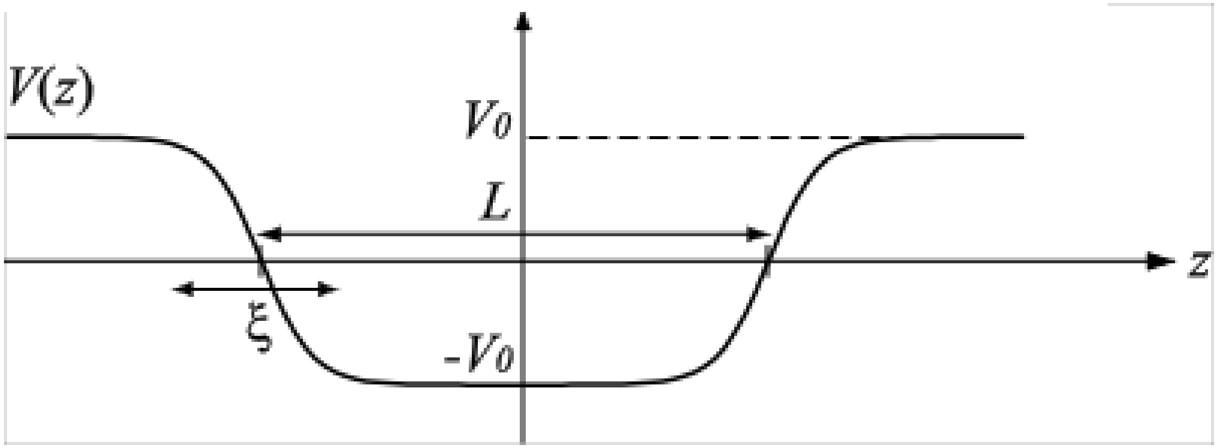
(valley splitting) < 1 K when L > 10 nm.

Hada and Eto, PRB **68**, 155322 (2003);
Hada and Eto, Phys. Stat. Sol. (c) **2**, 3035 (2005).

Empirical *spds** tight-binding model

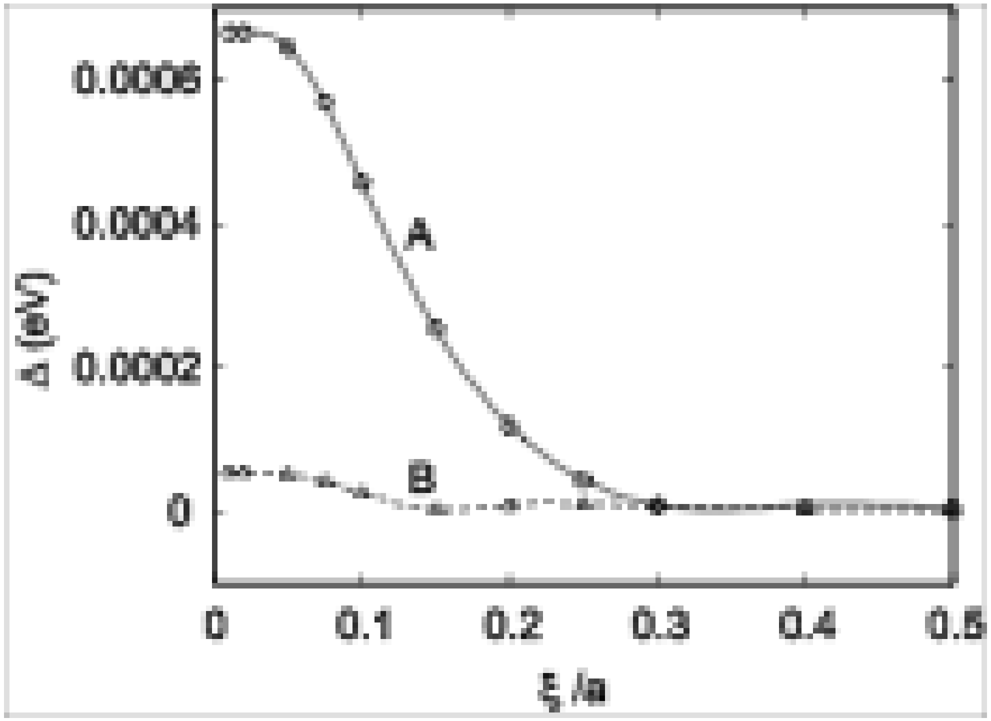
$$V(z) = V_0\{\tanh[(z-\frac{L}{2})/\xi] - \tanh[(z+\frac{L}{2})/\xi] + 1\}$$

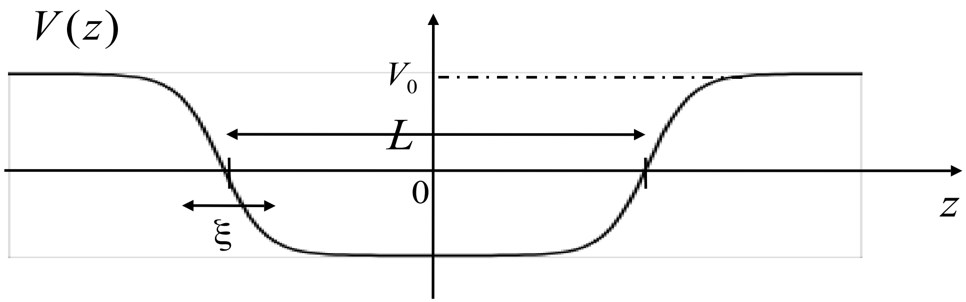




z: (0,0,1) direction; periodic boundary condition with period *a* in the other directions (only two valleys are considered).

- Split of degenerate valleys (energy difference between ground state and first excited state)





(A) $L = 8.25\,a = 4.5\text{nm}$

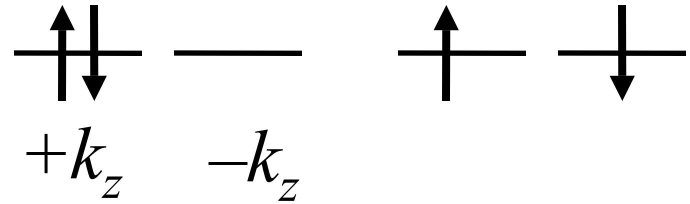
(B) $L = 16.25\,a = 8.8\text{nm}$

(II) Electron-electron interaction

- Coulomb integral

$$I_{\mathrm{C}} = \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \, |\psi_k(\boldsymbol{r}_1)|^2 \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} |\psi_{k'}(\boldsymbol{r}_2)|^2$$

$$= \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \, |F(\boldsymbol{r}_1)|^2 \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} |F(\boldsymbol{r}_2)|^2$$

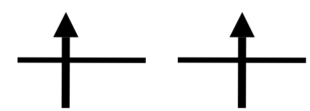


Intervalley integral is the same as intravalley one.

- Intervalley exchange integral

$$\iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \psi_k^*(\boldsymbol{r}_1) \psi_{k'}^*(\boldsymbol{r}_2) \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \psi_{k'}(\boldsymbol{r}_1) \psi_k(\boldsymbol{r}_2)$$

$$= \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \, \left|F(\boldsymbol{r}_1)\right|^2 \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \left|F(\boldsymbol{r}_2)\right|^2 e^{2ik_0(z_1 - z_2)} u_k^*(\boldsymbol{r}_1)\, u_{k'}^*(\boldsymbol{r}_2)\, u_{k'}(\boldsymbol{r}_1)\, u_k(\boldsymbol{r}_2)$$



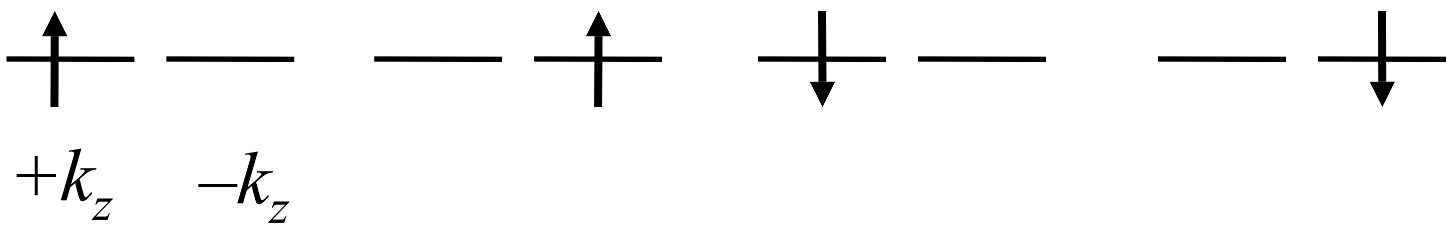
$$I_{\mathrm{ex}} / I_{\mathrm{C}} \sim 1/(k_0 L)^2 \sim (a/L)^2$$

Spin coupling is not effective!

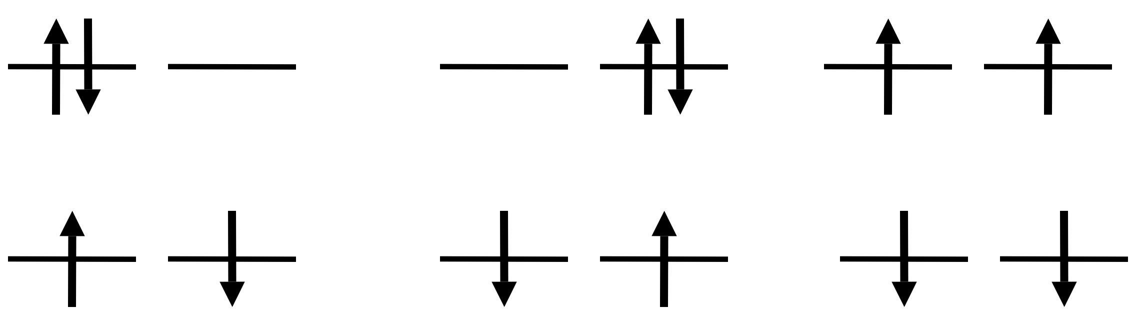
Summary of electronic states

"multivalley artificial atom"

- One electron in Si quantum dot: four-fold degeneracy



- Two electrons in Si quantum dot: six-fold degeneracy

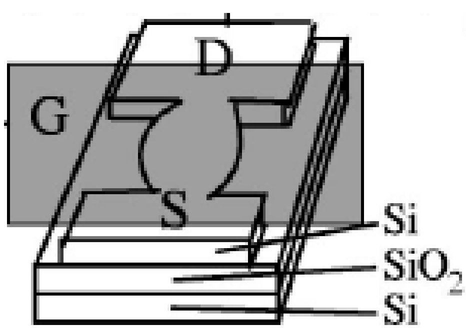


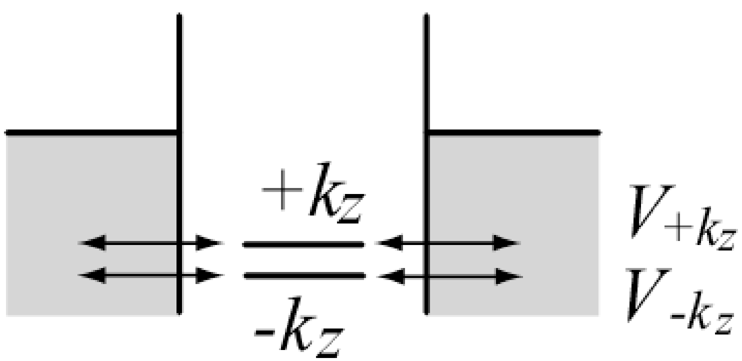
(three spin-singlets and one spin-triplet)

5.3. Kondo effect in Si quantum dots

- A quantum dot and two leads fabricated on Si-MOS
  [experiment] Rokhinson *et al*., PRB **60**, R16319 (1999).

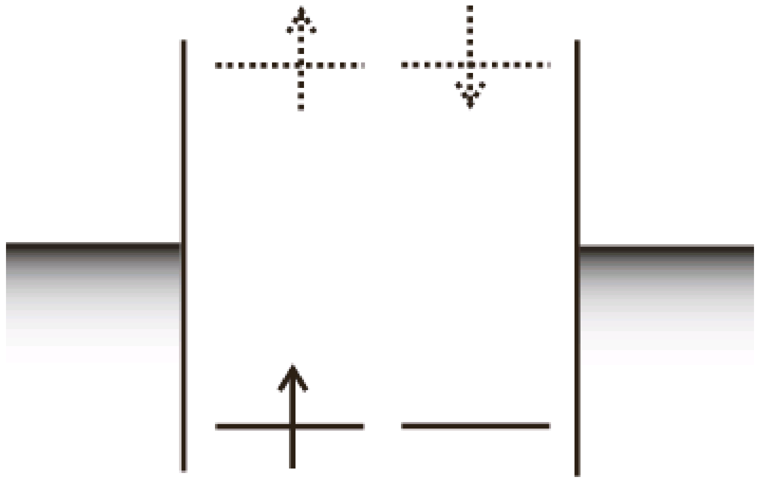
- Valley index ($+k_z$ or $-k_z$) is conserved in tunneling processes (barrier thickness >> a)
  → Two channels in the leads



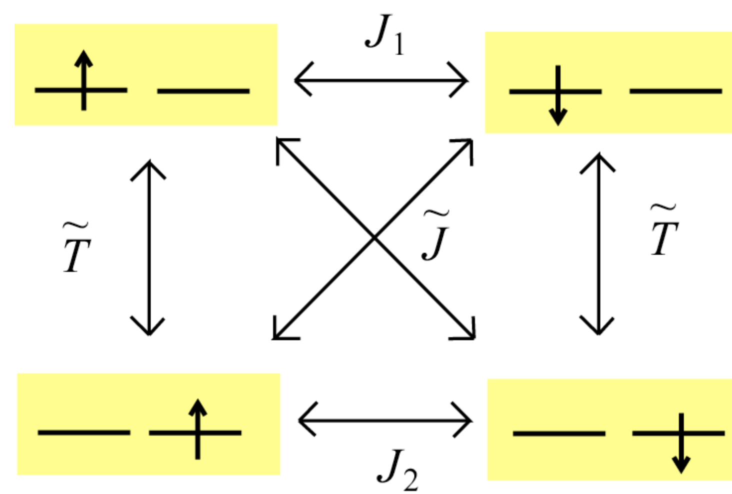


5.3.1. SU(4) Kondo effect with one electron

Coulomb blockade with one electron

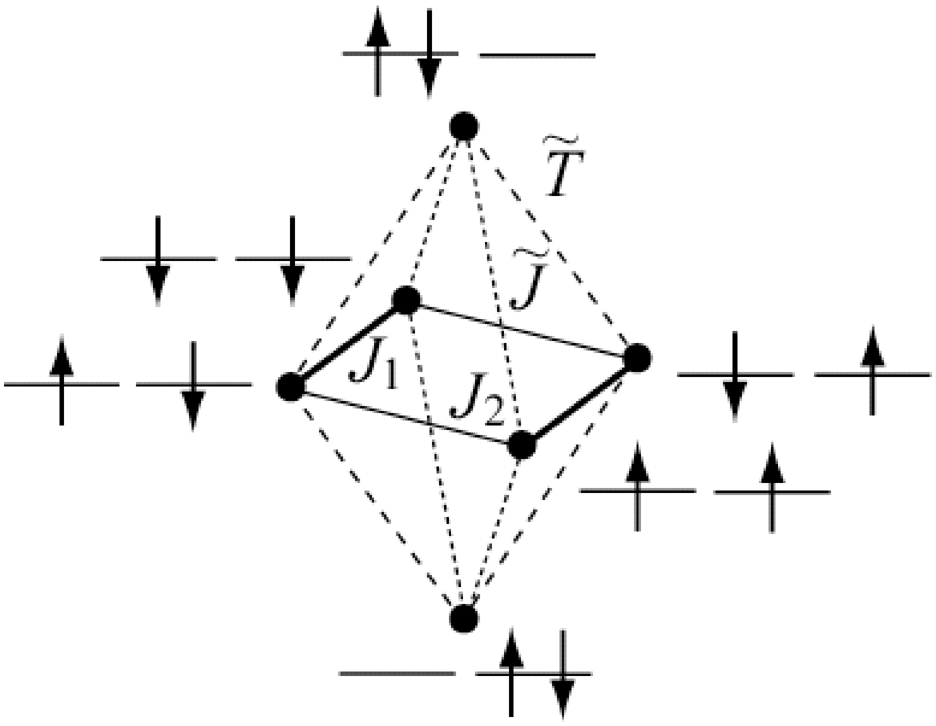


- SU(4) Kondo effect results in large T_K.



5.3.2. Kondo effect with two electrons

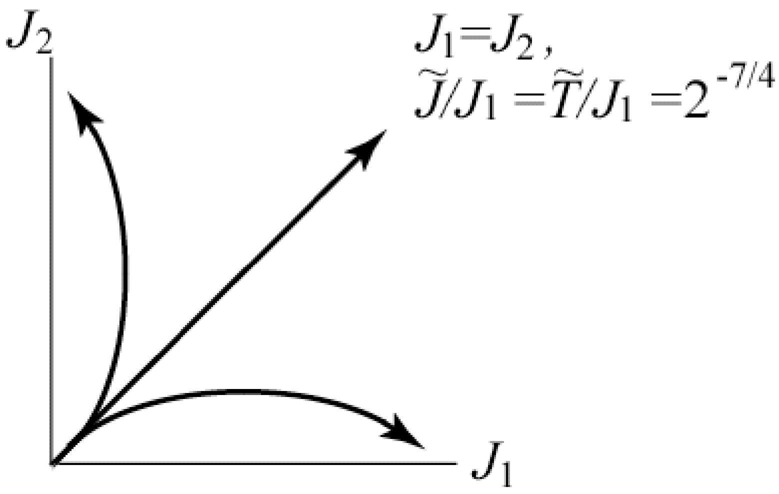
- Six-fold degeneracy in Coulomb blockade with two electrons when exchange integral < T_K



$$J_1 = V_k^2 / \tilde{E}_C,$$
$$J_2 = V_{k'}^2 / \tilde{E}_C,$$
$$\tilde{J} = \tilde{T} = V_k V_{k'} / \tilde{E}_C$$
$$\left(1 / \tilde{E}_C = 1 / E^+ + 1 / E^-\right)$$

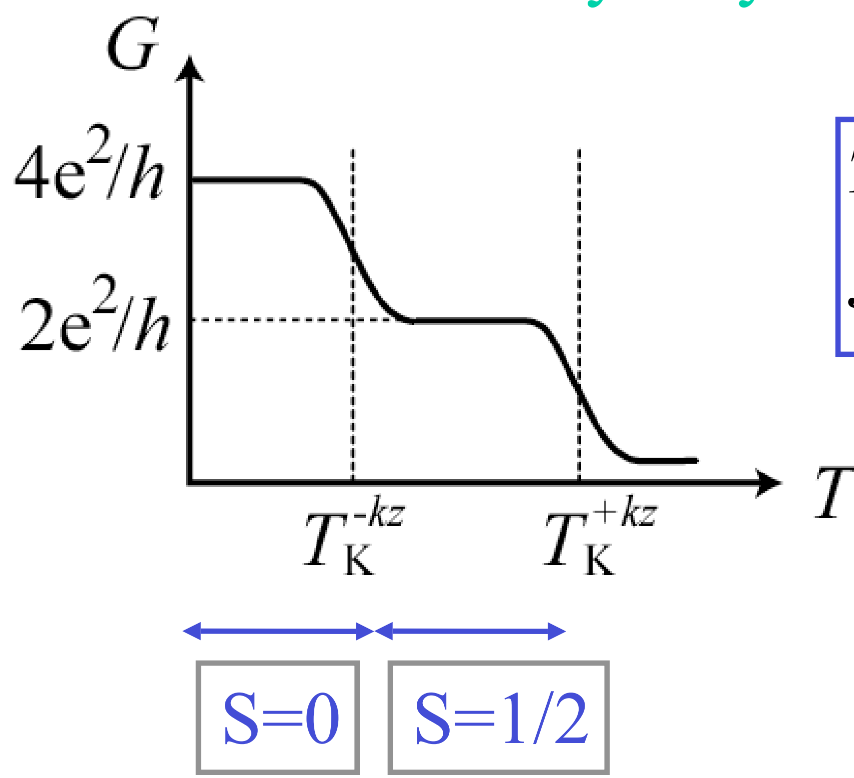
Scaling analysis

$$
\begin{cases}
dJ_1/\nu d\ln D = -2(J_1^2 + 2\tilde{J}\tilde{T}) \\
dJ_2/\nu d\ln D = -2(J_2^2 + 2\tilde{J}\tilde{T}) \\
d\tilde{J}/\nu d\ln D = -(J_1+J_2)\tilde{J}/2 - (J_1+J_2)\tilde{T} - T\tilde{J} \\
d\tilde{T}/\nu d\ln D = -(J_1+J_2)\tilde{T}/2 - (J_1+J_2)\tilde{J} - T\tilde{T} \\
dT/\nu d\ln D = -2\left(\tilde{J}^2 + \tilde{T}^2\right)
\end{cases}
$$



A new fixed point of "underscreened Kondo" is unstable against asymmetry.

- When $V_k = V_{k'}$, an underscreening Kondo effect with large Kondo temperature.
- When $V_k \neq V_{k'}$, two independent SU(2) Kondo effects; spin 1/2 in a valley is screened by the conduction electrons in the same valley only.



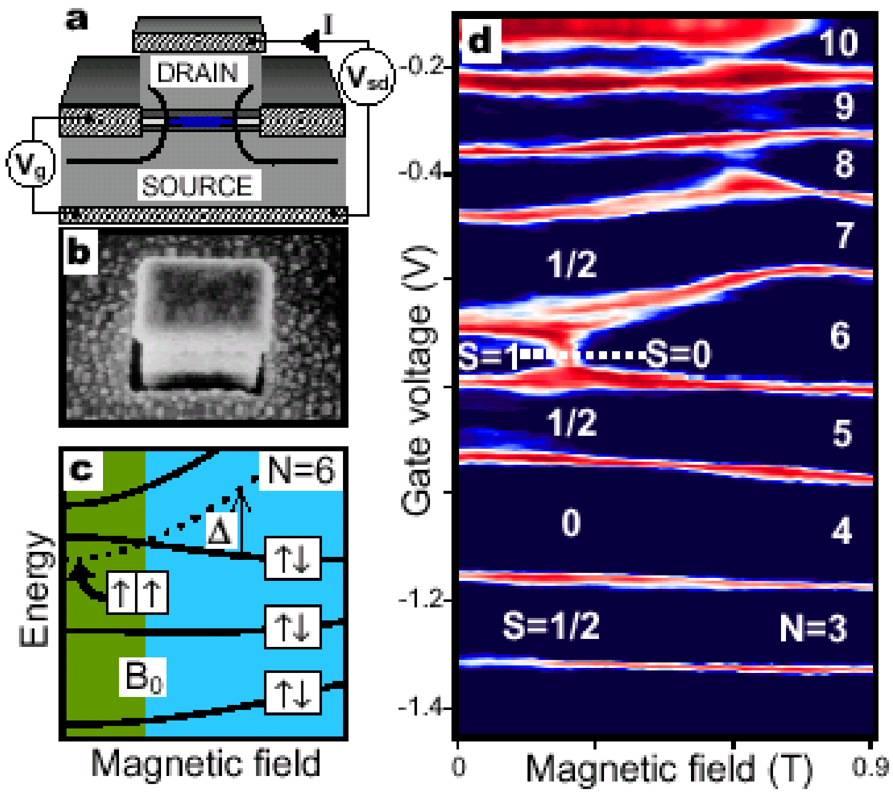
$$T_K^{\pm k_z} = D \exp\left(-1/2\nu J_{\pm k_z}\right)$$

$$J_{\pm k_z} = V_{\pm k_z}^2 \left(1/E_+ + 1/E_-\right)$$

- Contrast to singlet-triplet Kondo effect which has a stable fixed point

  cf. Pustilnik and Glazman, PRL (2000).

$$|S=0,S_z=0\rangle,$$
$$|S=1,S_z=1\rangle,|1,0\rangle,|1,-1\rangle$$



- Four-fold degeneracy when exchange interaction is larger than level spacing.

5.4. Conclusions

- Theoretical studies of electronic states and Kondo effect in Si quantum dots
- Energy levels are degenerate, reflecting equivalent valleys
- Intervalley exchange interaction is not effective when dot size is much larger than *a*.
- SU(4) Kondo effect for an electron with four-fold degeneracy
- Two-stage Kondo effect for two electrons with six-fold (three spin-singlet and one triplet) degeneracy

Silicon:

- Valley splitting usually exists, but controllable.

  Tanashina *et al*., PRL (2006).

Carbon nanotubes:

- SU(4) Kondo effect by valley degeneracy

  Jarillo-Herrero *et al*., Nature **434**, 484 (2005).

- Not our case with two electrons

  Exchange interaction works in carbon nanotubes.

$$I_{\mathrm{ex}} / I_{\mathrm{C}} \sim 1/(k_0 L)^2 \sim (a/L)^2$$ (L: radius of nanotube)

Related theory: two electrons in double quantum dots:
Galpin, Logan, Krishnamurthy, PRL (2005).