

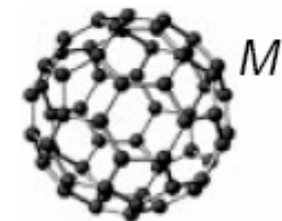
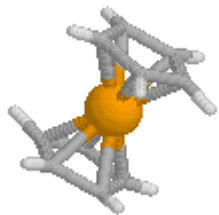


Institut für Theoretische Physik
Universität Würzburg
and
The Abdus Salam International Centre
for Theoretical Physics



M.N.Kiselev

Kondo Shuttling



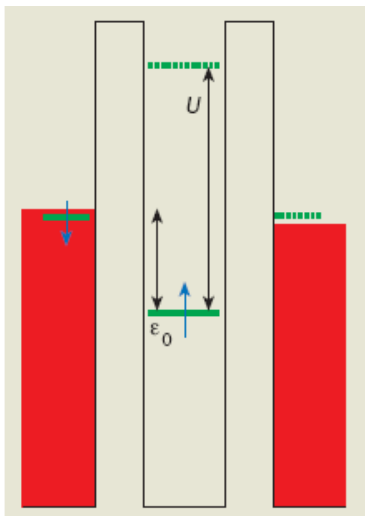
Workshop on Quantum Pumping, Haifa, January 8, 2007

Single orbital level coupled to two leads



$$H = H_{leads} + H_{tun} + H_{dot}$$

$$H_{leads} = \sum_{k,\sigma\alpha=L,R} [\epsilon_k - \mu_\alpha] c_{k,\sigma\alpha}^\dagger c_{k,\sigma\alpha}$$



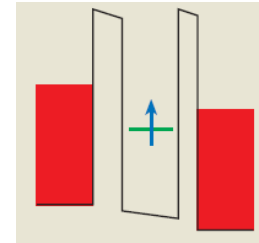
$$H_{tun} = \sum_{k,\sigma\alpha} [V_\alpha(t) c_{k,\sigma\alpha}^\dagger d_\sigma + H.c.]$$

$$H_{dot} = \sum_{\sigma} \epsilon_0 d_\sigma^\dagger d_\sigma + U(n - N)^2$$

Tunneling width

$$\Gamma_\alpha(t) = \pi \rho |V_\alpha|^2(t)$$

Single orbital level coupled to two leads



Time-dependent Glazman-Raikh rotation

$$\begin{pmatrix} c_{k\sigma L} \\ c_{k\sigma R} \end{pmatrix} = U_t \begin{pmatrix} c_{k\sigma+} \\ c_{k\sigma-} \end{pmatrix} \quad U_t = \begin{pmatrix} \cos \theta_t & -\sin \theta_t \\ \sin \theta_t & \cos \theta_t \end{pmatrix}$$

$$\tan \theta_t = \left| \frac{V_R(t)}{V_L(t)} \right| \quad |V|^2(t) = |V_L|^2(t) + |V_R|^2(t)$$

$$H_{Berry} = \sum_{k, \sigma \gamma = \pm} (c_{k, \sigma+}^\dagger + c_{k, \sigma-}^\dagger) \underbrace{\left[-i U_t^{-1} \frac{\partial U_t}{\partial t} \right]}_{a_t} \begin{pmatrix} c_{k, \sigma+} \\ c_{k, \sigma-} \end{pmatrix}$$

Gauge potential

$$a_t = \frac{d\theta_t}{dt} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

Adiabatic current and pumped charge per cycle at T=0

$$I_\sigma = \frac{e}{2\pi} \left[-\frac{d\theta_t}{dt} \sin(2\theta_t) \sin(2\delta_\sigma(t)) + \frac{d\delta_\sigma}{dt} \cos(2\theta_t) \right]$$

Scattering phase shifts

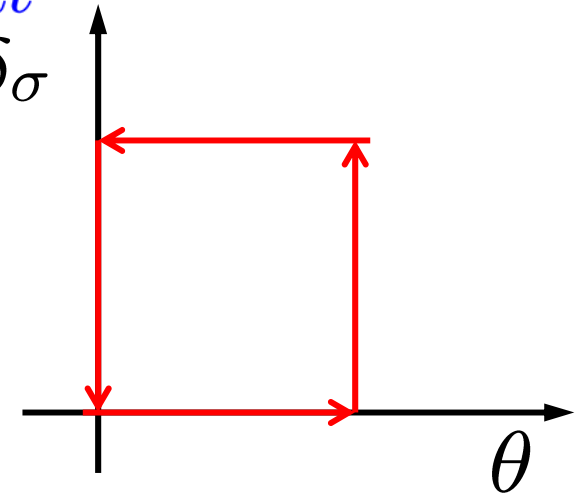
at the Fermi level in the leads

$$Q_\sigma = \oint dt I_\sigma(t) = \frac{e}{2\pi} \oint dt (1 - T_\sigma) \frac{d\Upsilon_\sigma}{dt}$$

$$T_\sigma = \sin^2(2\theta_t) \sin^2 \delta_\sigma(t)$$

$$\Upsilon_\sigma = \arctan[\cos^2(2\theta_t) \tan \delta_\sigma(t)]$$

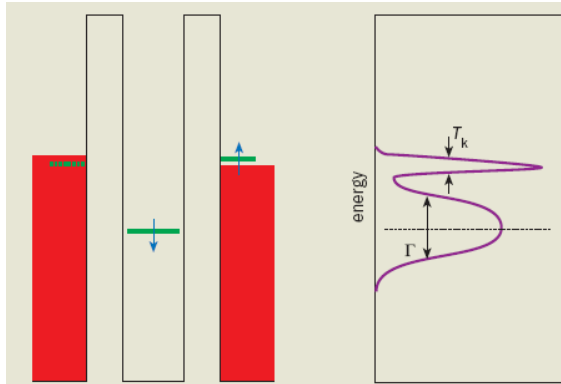
$$Q_\sigma = \frac{e}{2\pi} \oint (\cos(2\theta) d\delta_\sigma - \sin(2\theta) \sin(2\delta_\sigma) d\theta)$$



Adiabaticity $\hbar\Omega \ll \min[\Gamma(t)]$

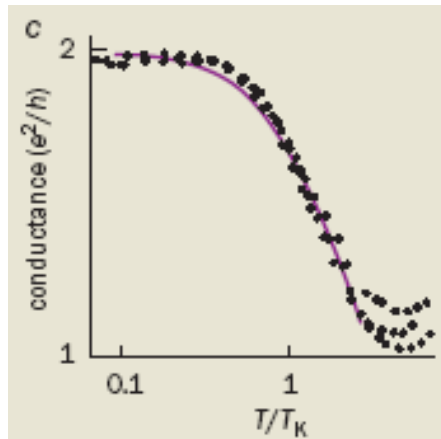
M.Büttiker et al, 1994

Adiabatic pumping at the Kondo regime



$$\delta_\sigma \rightarrow \frac{\pi}{2} \quad \text{Nozieres Fermi Liquid regime}$$

$$T_K = \sqrt{(\Gamma_L + \Gamma_R)U/\pi} \exp \left[-\frac{\pi U}{4(\Gamma_L + \Gamma_R)} \right]$$



Pumped charge

$$Q_c = Q_\uparrow + Q_\downarrow = 0$$

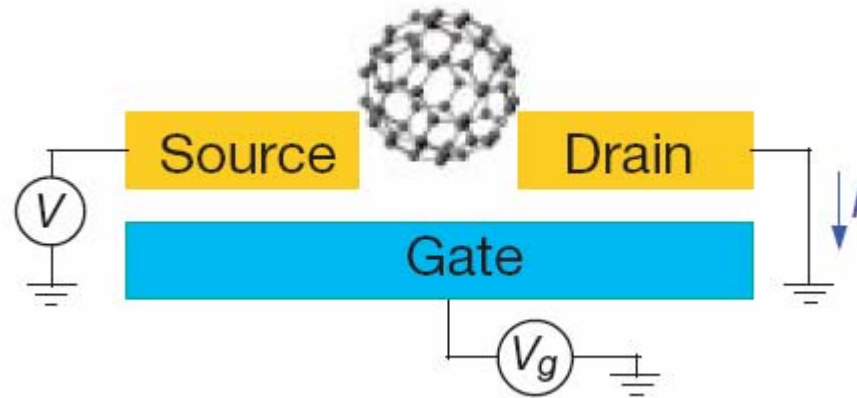
Pumped spin

$$Q_s = Q_\uparrow - Q_\downarrow \neq 0$$

Kondo Pump = Resonance Spin Diode

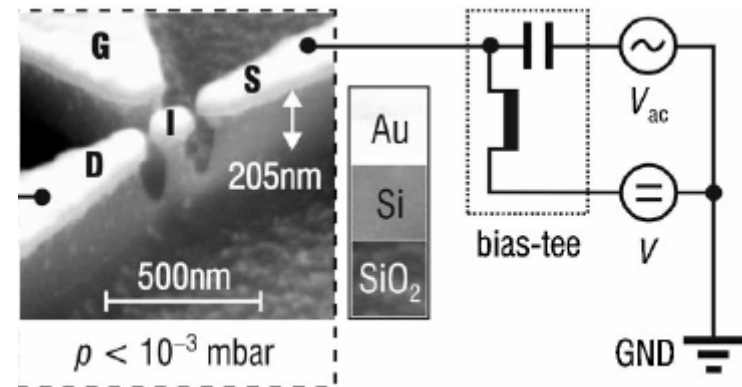
What if $\Gamma(t)$ is due to a nanomechanics?

Molecular Transistor



H.Park et al, Nature 2000

Nano-Pendulum

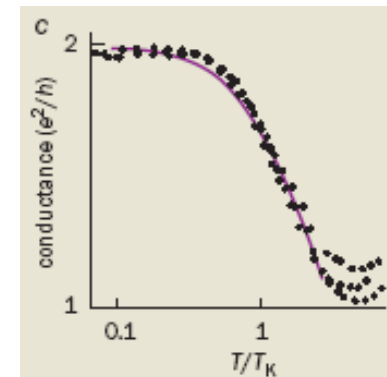
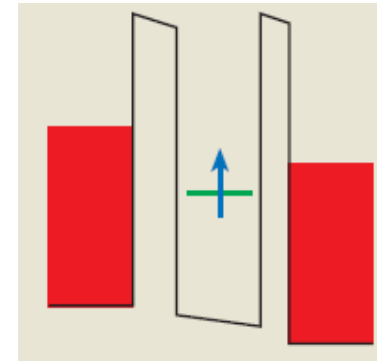
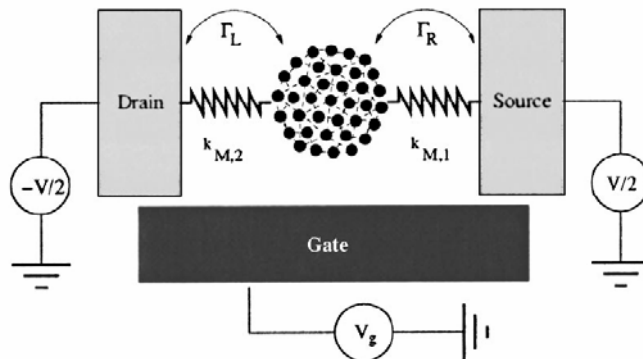


D.Sheible and R.Blick 2004

NanoElectroMechanical Pump = Shuttle

Why do we look for the Kondo effect in nano-devices ?

- The Kondo effect makes it easier for states belonging to the two opposite electrodes to mix
- Reasonably high Kondo temperatures > 1 K
- SETs are highly controllable (by bias, magnetic field etc) devices





Keeping in mind **Pumping** ...

I will speak about **Shuttling**.

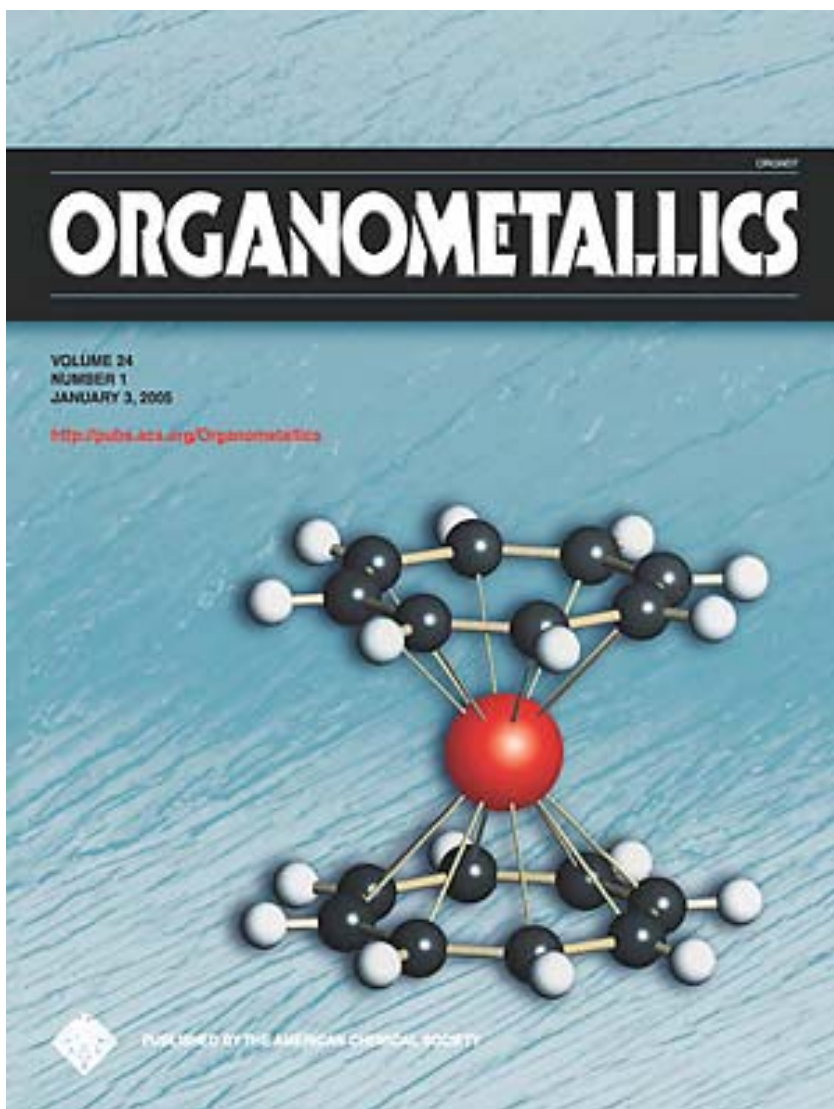
How to make the Kondo effect work
in the Nanoelectromechanical devices?

How is the KE influenced by the NEM?

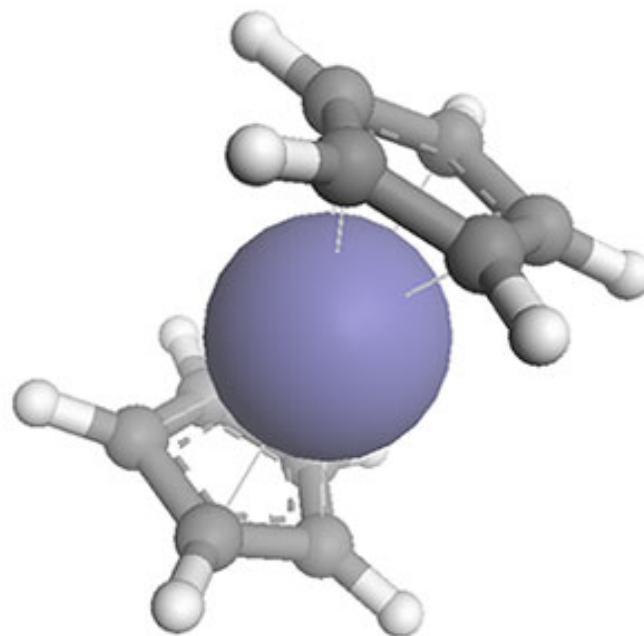
- the nano-device changes its shape in the process of the tunneling
- the nano-device is nano-machined by external periodic force

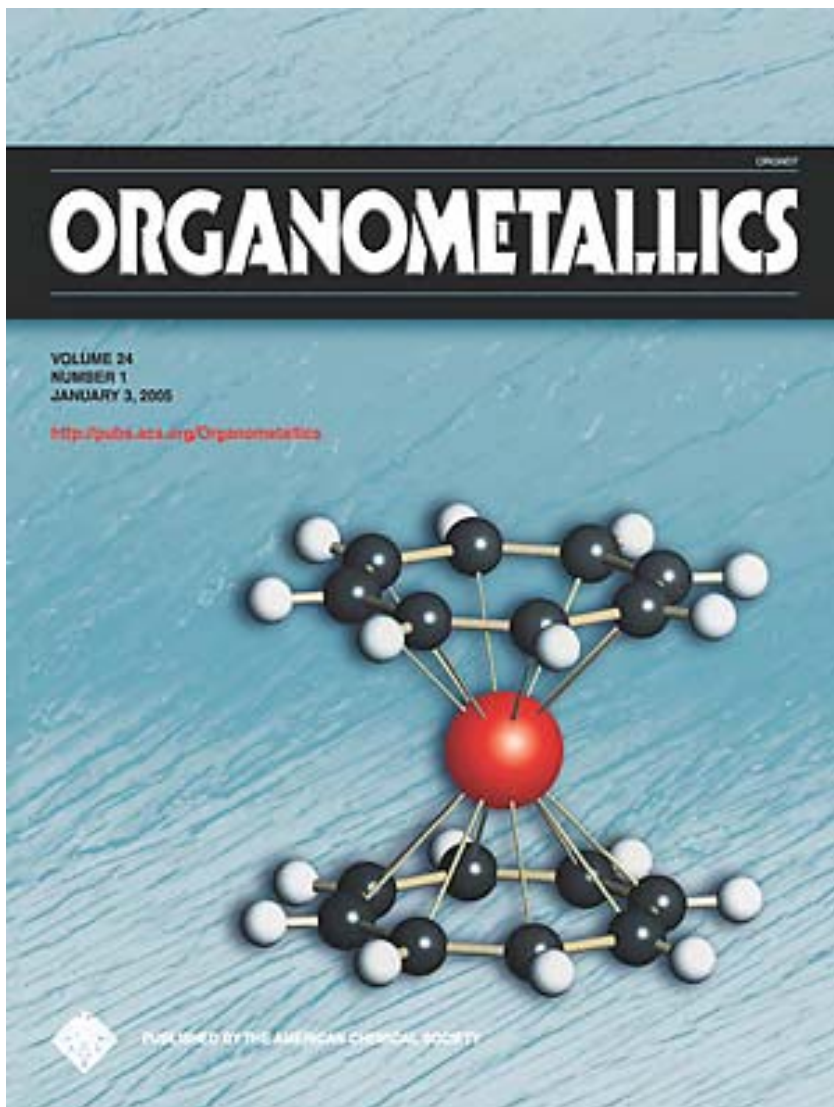
K.Kikoin, MK and M.R.Wegewijs, PRL 2006

MK, K.Kikoin, R.Shekhter and V.Vinokur, PRB 2006



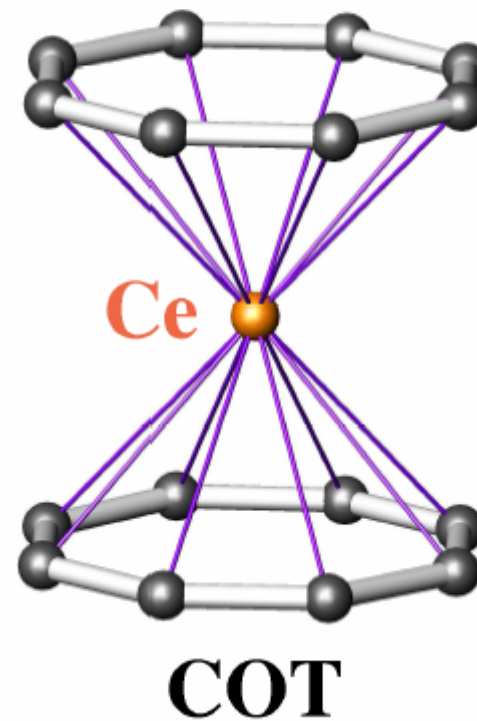
Ferrocene $Fe(C_5H_5)_2$



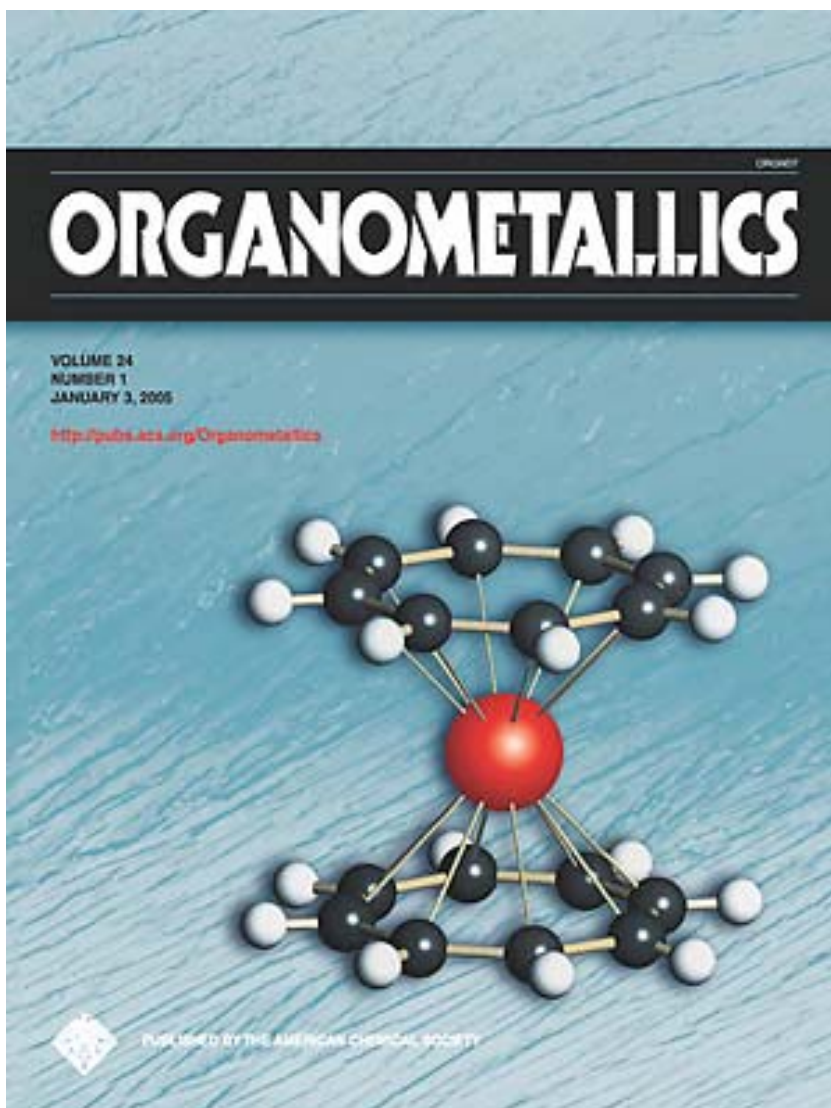


Cerocene $Ce(C_8H_8)_2$

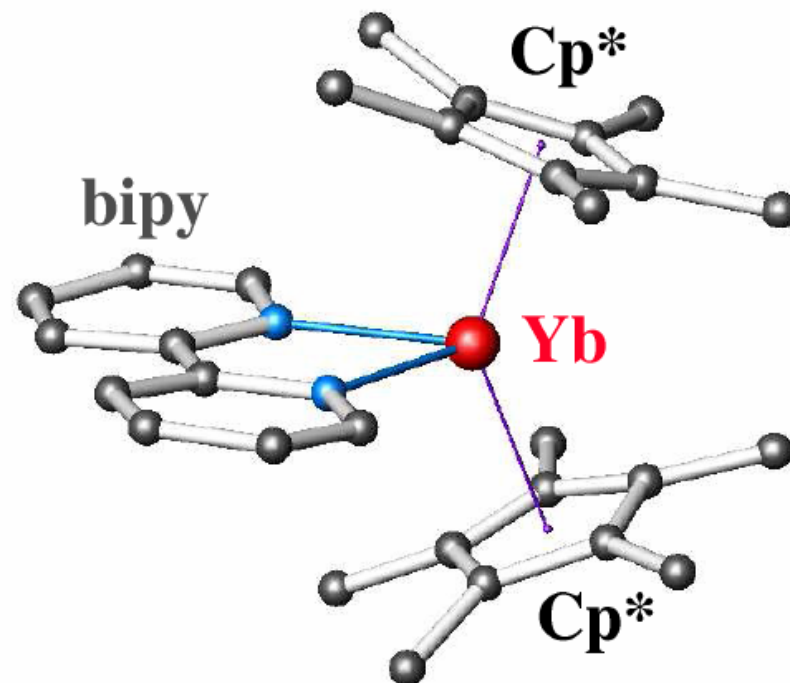
$Ce(COT)_2$



COT = C₈H₈

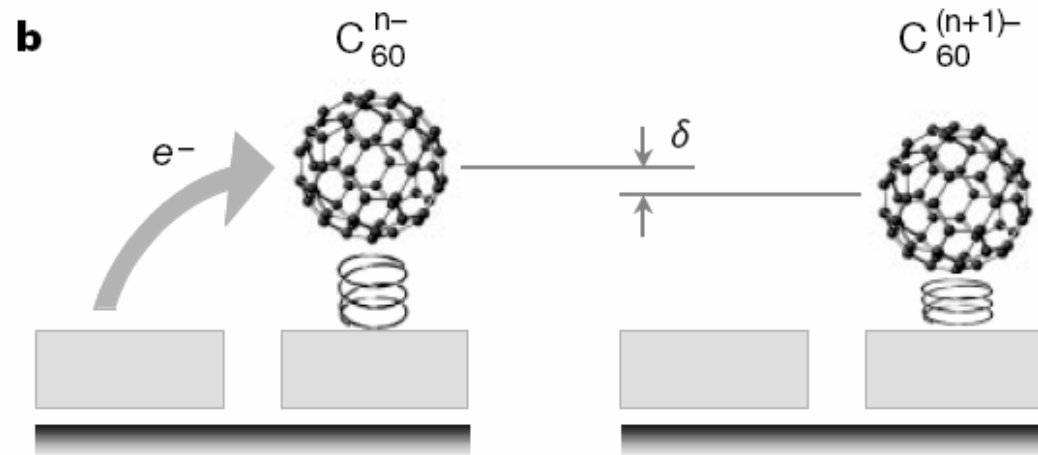
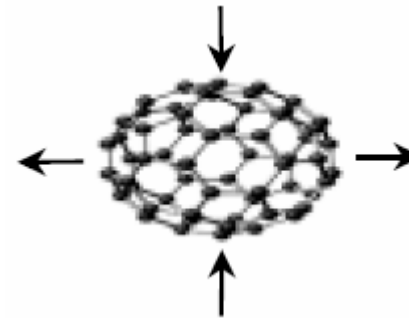
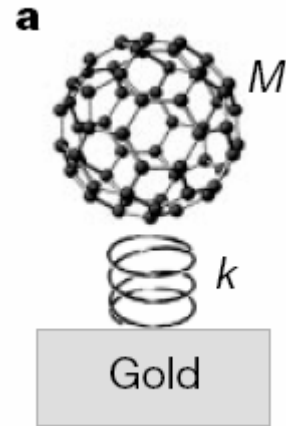
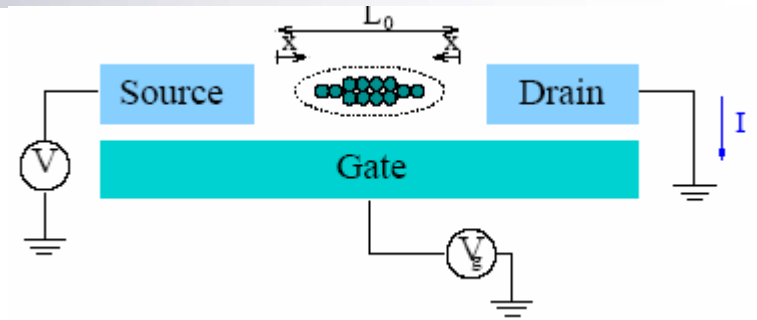


Ytterbocene

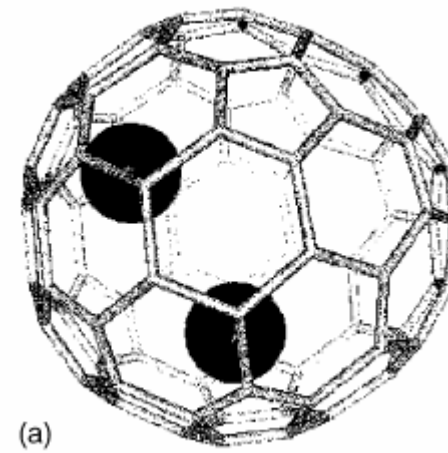
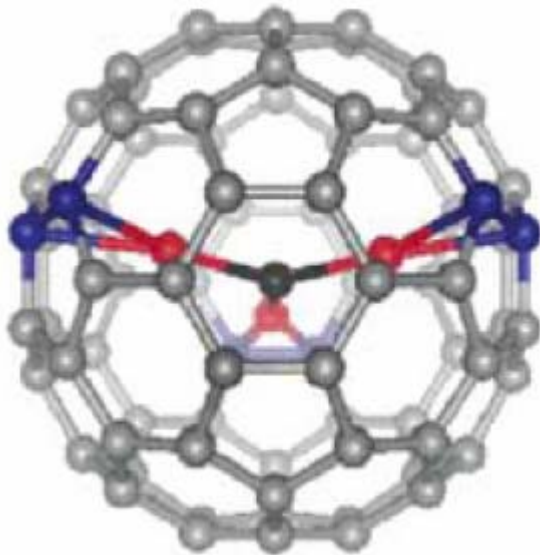
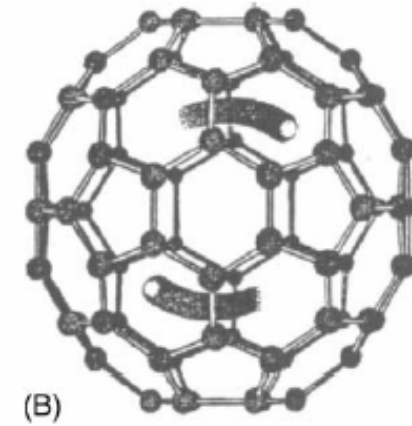
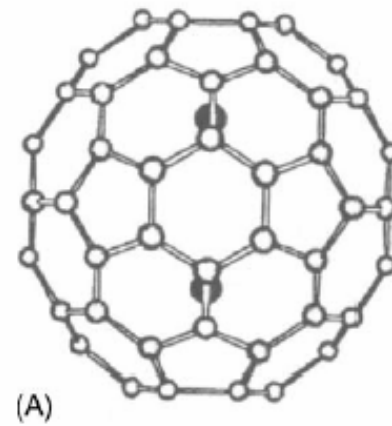
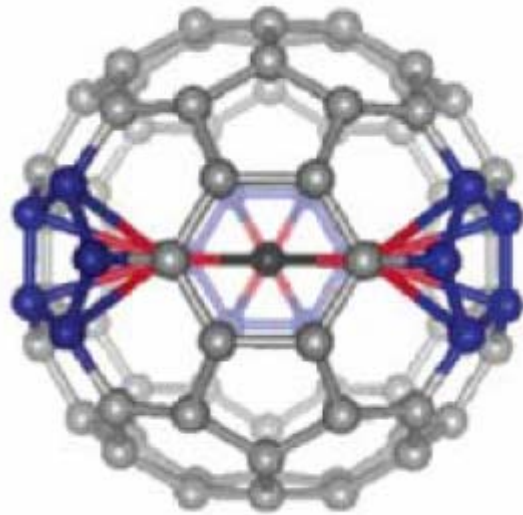


$\text{Cp}^* = \text{C}_5\text{Me}_5$, $\text{bipy} = (\text{NC}_5\text{H}_4)_2$

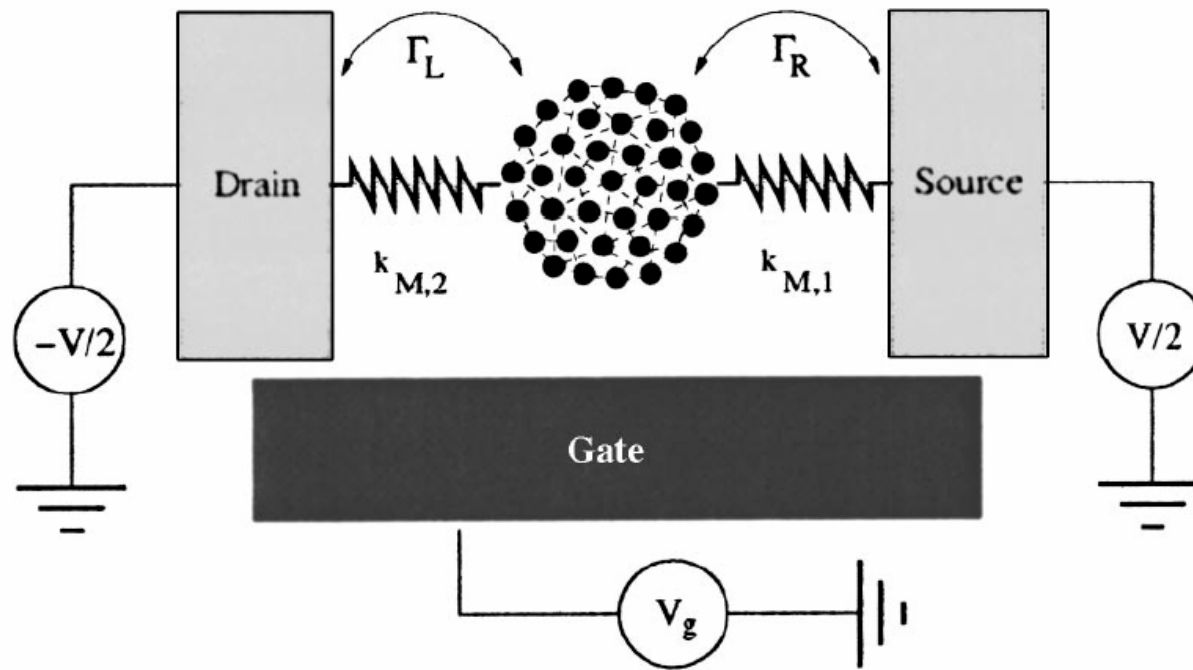
Fullerenes



Transition metals inside fullerenes



Transport through molecular transistors





Q: Whether phonons support or destroy Kondo effect?

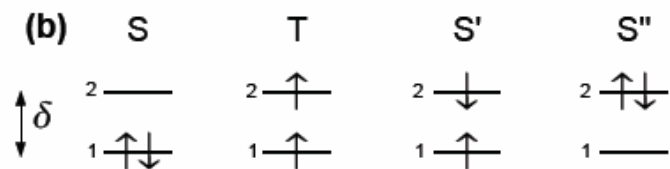
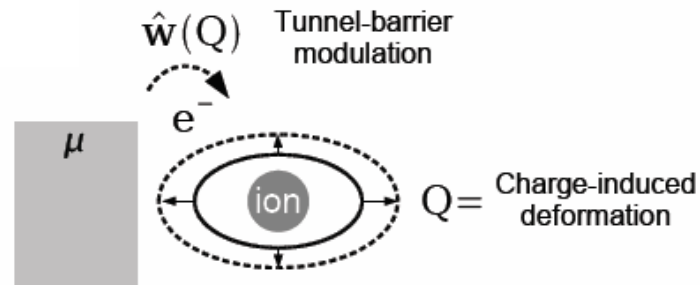
A: Usually they destroy it due to the energy transfer and the decoherence effects.

Q: Can phonons assist a resonance tunneling?

A: Yes, they can do it through dynamical symmetries.

Phonons + Kondo = "Phondo"

Effective model



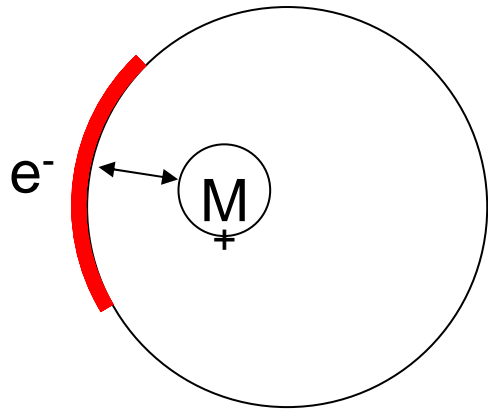
$$H = H_{mol} + H_{res} + H_{tun}$$

$$H_{mol} = H_Q^{(N)} + H_Q^{(N+1)} + H_Q^{(N-1)} + T_n$$

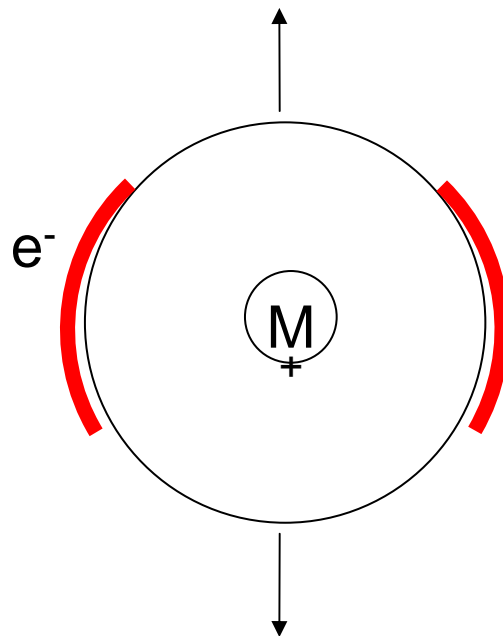
$$H_{res} + H_{tun} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \hat{w}_Q \sum_{k\mu\sigma} \left(\tilde{d}_{\mu\sigma}^\dagger c_{k\sigma} + H.c. \right)$$

cage MO = localized

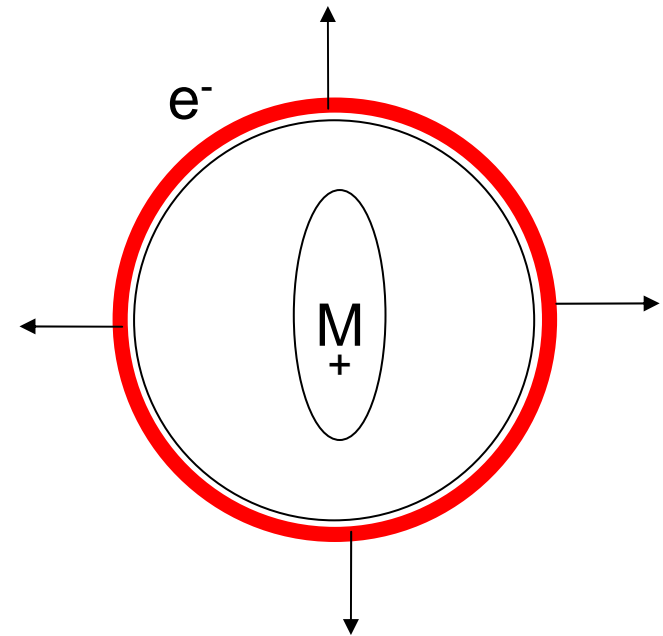
cage MO = delocalized



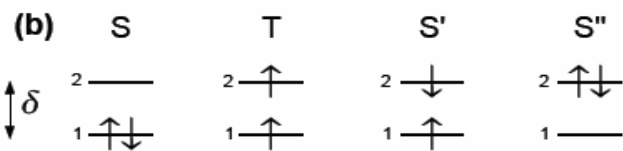
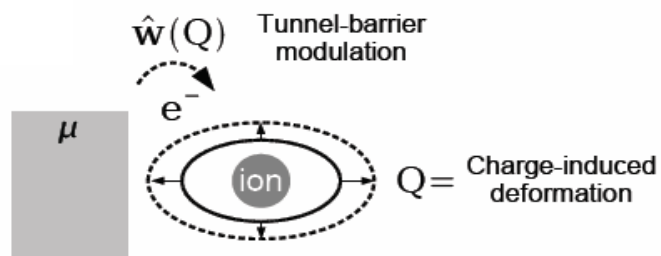
dipolar



quadrupolar



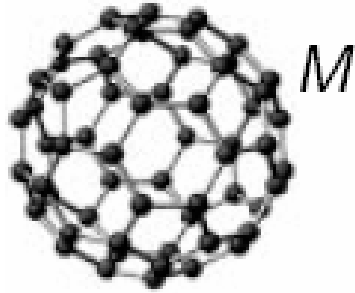
breathing



$$\Delta \equiv E_T - E_S = \delta - I > T_K$$

Triplet
Singlet
Exchange

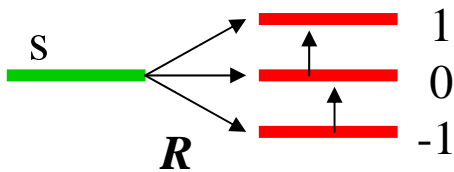
TMOC = Transition Metal + Organic Complex (cage)



$$H_{mol}^{(N)} = \sum_{\Lambda=S, T_0, T_{\pm}} E_{\Lambda}(Q) |\Lambda\rangle \langle \Lambda|$$

Singlet Triplet

Assumption: even electron occupation number



Singlet is a ground state

SO(4) symmetry

$$H_{tun} = \hat{w}(Q) \sum_k \sum_{\Lambda \gamma \sigma} [|\Lambda\rangle \langle \gamma| c_{k\sigma} + H.c.]$$

$$H_{eff} = H_{res} + \frac{1}{2} \Delta S^2 + \hat{J}_S \mathbf{S} \cdot \mathbf{s} + \hat{J}_R \mathbf{R} \cdot \mathbf{s} + \frac{\Omega}{2} P^2$$

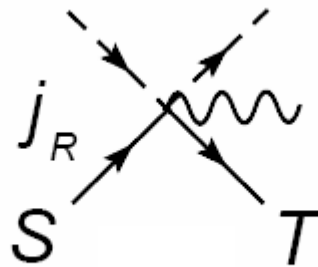
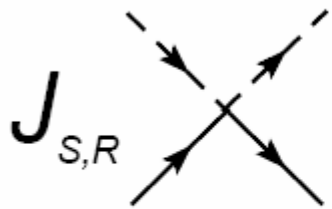
Local phonon can be emitted or absorbed in a co-tunneling processes

The main source of phonon emission/absorption is the tunneling rate

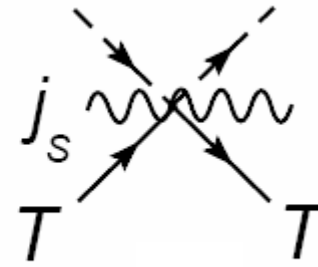
Vibration assisted tunneling

$$H_{eff} = H_{res} + \frac{1}{2}\Delta S^2 + \hat{J}_S S \cdot s + \hat{J}_R R \cdot s + \frac{\Omega}{2}P^2$$

$$\hat{J}_S(Q) = J_S + j_S Q^2, \quad \hat{J}_R(Q) = J_R + j_R Q$$



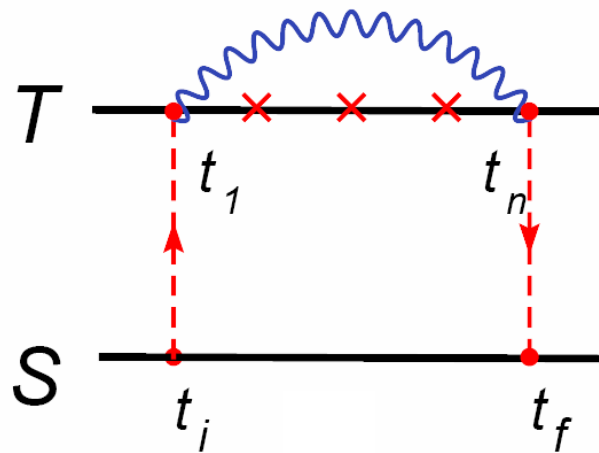
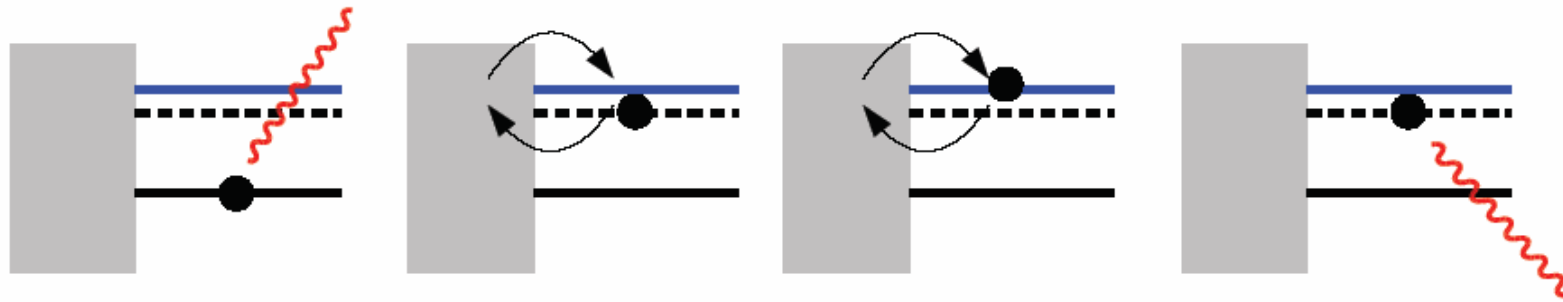
single phonon



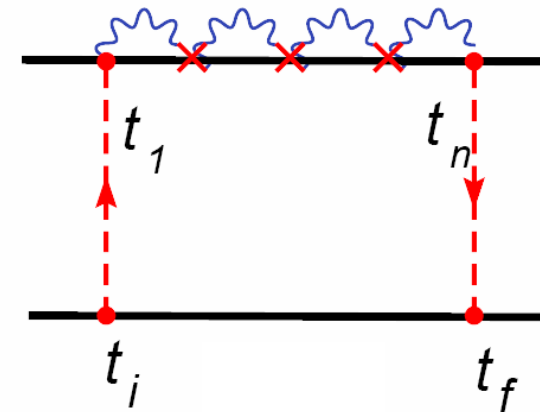
two-phonon

$$j_S \ll j_R$$

Phonon assisted processes



single-phonon



two-phonon

Single phonon processes

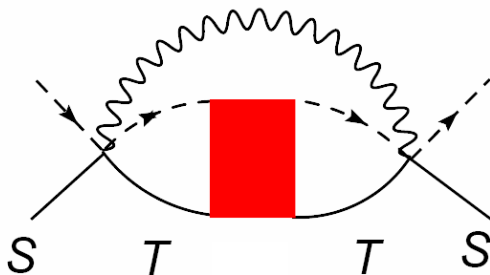


$$\gamma^{(1)} \sim j_R^2 \int \frac{d\epsilon}{2\pi} \int \frac{d\omega}{2\pi} \tanh\left(\frac{\epsilon}{2T}\right) \text{Im}G^R(\epsilon) \text{Re}\bar{G}^R(\omega) \text{Im}D^R(\epsilon-\omega) \coth\left(\frac{\epsilon-\omega}{2T}\right)$$



$$\gamma^{(1)} = \gamma^{(2)} \sim \rho j_R^2 \log\left(\frac{D}{\max[T, |\Delta - \Omega_0|]}\right)$$

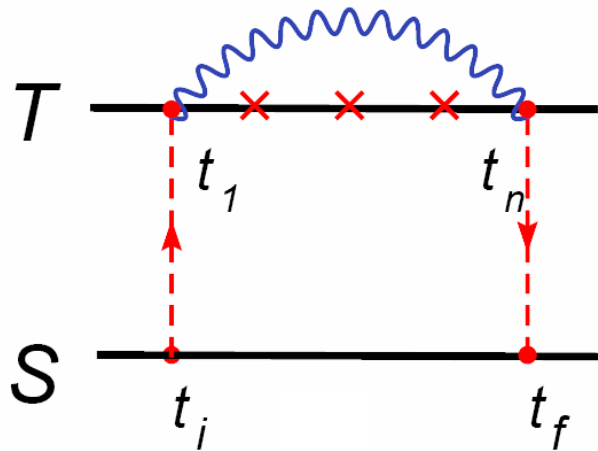
$$\gamma^{(2)} \sim j_R^2 \int \frac{d\epsilon}{2\pi} \int \frac{d\omega}{2\pi} \tanh\left(\frac{\epsilon}{2T}\right) \text{Im}G^R(\epsilon) \text{Re}\bar{G}^R(\omega) \text{Im}D^R(-\epsilon-\omega) \coth\left(\frac{\epsilon+\omega}{2T}\right)$$



Summation of “parquet” diagrams

$$\gamma_1 \sim j_R^2 \int \frac{d\epsilon}{2\pi} \coth\left(\frac{\epsilon}{2T}\right) \left[\text{Re} \left[\frac{\Pi(-\epsilon)}{1 - J_0^T \bar{\Pi}(-\epsilon)} \right]^R \text{Im}D^R(\epsilon) + \text{Re}D^R(-\epsilon) \text{Im} \left[\frac{\Pi_i(\epsilon)}{1 - J_0^T \bar{\Pi}(\epsilon)} \right]^R \right]$$

Single phonon processes



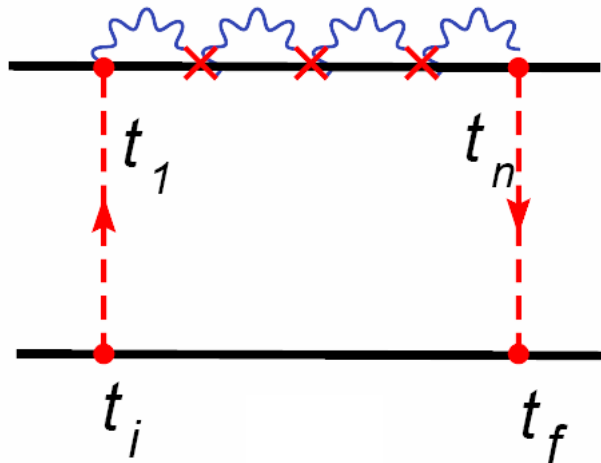
$$\gamma_1 \sim (j_R)^2 \rho \left[\frac{\log \left(\frac{D}{\max[T, |\Delta - \Omega|]} \right)}{1 - J_S A \rho \log \left(\frac{D}{\max[T, |\Delta - \Omega|]} \right)} \right]$$

$$T_K^{(1)} \sim D \exp \left(-\frac{1}{A \rho J_S} \right)$$

Messages:

- Single phonon processes assist the Kondo tunneling
- Kondo temperature does not depend on the phonon coupling
- Differential conductance is logarithmically enhanced approaching the Kondo regime

Two-phonon processes



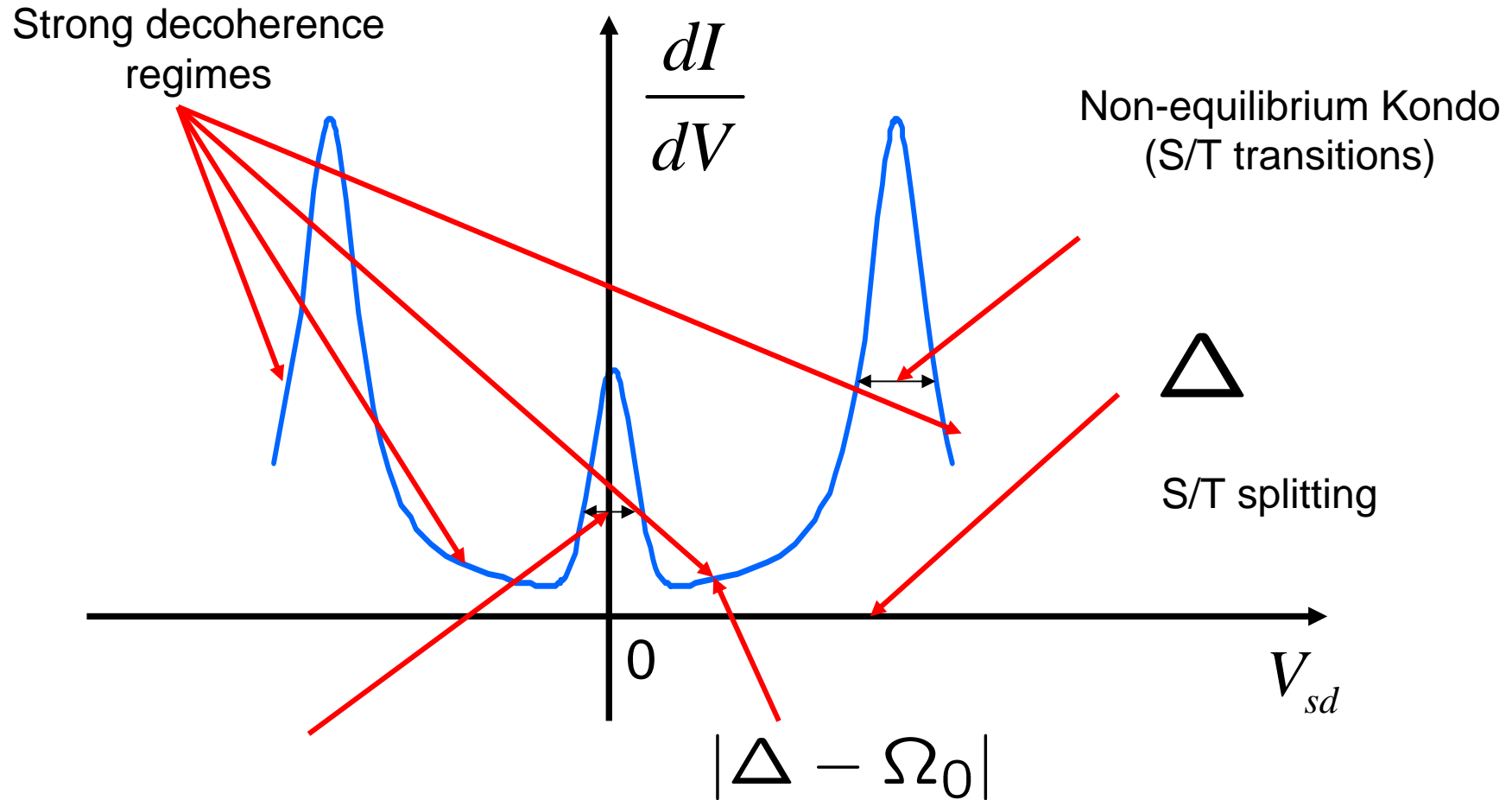
$$\gamma_2 \sim (j_R)^2 \rho \left[\frac{\log \left(\frac{D}{\max[T, |\Delta - \Omega|]} \right)}{1 - j_S A' \rho \log \left(\frac{D}{\max[T, |\Delta - \Omega|]} \right)} \right]$$

$$T_K^{(2)} \sim D \exp \left(-\frac{1}{A' \rho j_S} \right) \ll T_K^{(1)}$$

Messages:

- Two-phonon processes also assist the Kondo tunneling, **however**
- Kondo temperature **depends** on the phonon coupling
- The two phonon scenario leads to much smaller Kondo temperatures

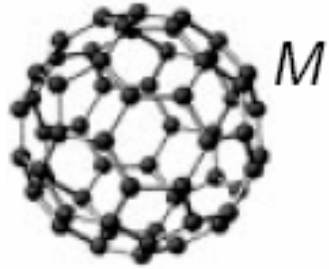
Differential Conductance



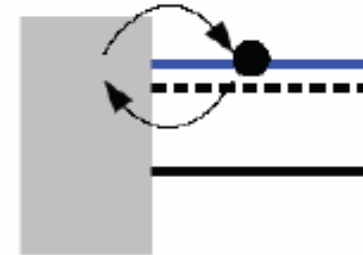
Equilibrium Kondo temperature
(triplet state)

**Log-scaling of peaks is a manifestation
of the Kondo effect**

A resonance condition



$$|\Omega_0 - \Delta| \ll T_K$$

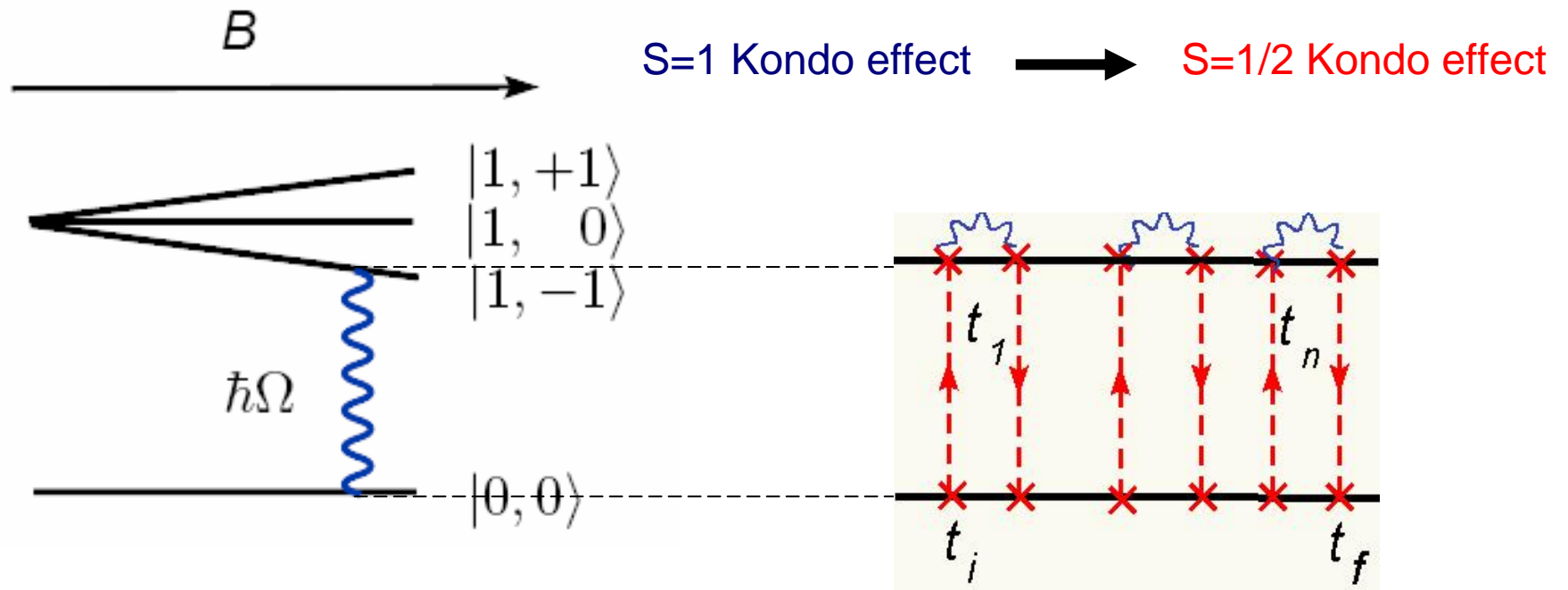


... narrows a group of the TMOC with “Phondo”.

What happens if $T_K < |\Omega_0 - \Delta| \ll \Delta$?

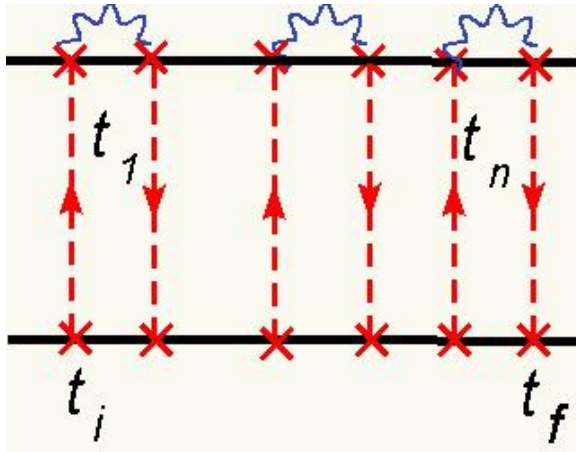
Fine tuning tool is necessary to control the resonance

Magnetic Field Effects



Magnetic field as a fine tuning tool

Single-phonon processes in magnetic field



$$\gamma_B \sim \left[\frac{(j_R)^2 \rho \log \left(\frac{D}{\max[T, B, |\Delta - \Omega - B|]} \right)}{1 - (j_R A_{B\rho})^2 \log^2 \left(\frac{D}{\max[T, B, |\Delta - \Omega - B|]} \right)} \right]$$

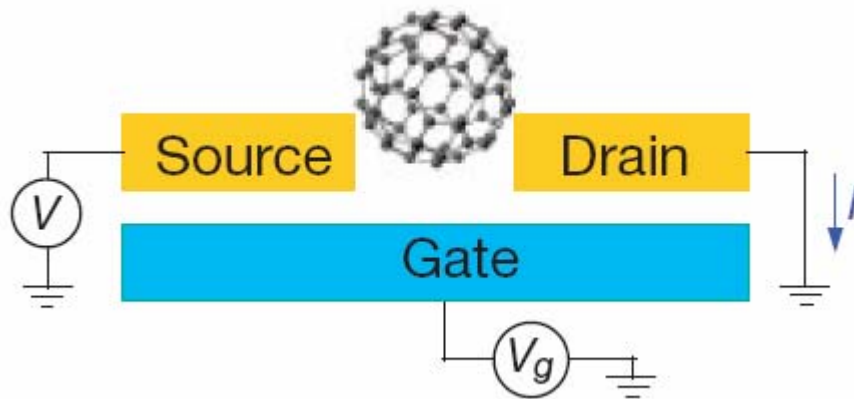
$$T_K^{(2)} \ll T_K^{(B)} \sim D \exp \left(-\frac{1}{A_{B\rho} j_R} \right) \ll T_K^{(1)}$$

Messages:

- Single-phonon processes assist the Kondo tunneling, **however**
- Kondo temperature **depends** on the phonon coupling
- Magnetic field provides a tool for the fine tuning of the TMOC

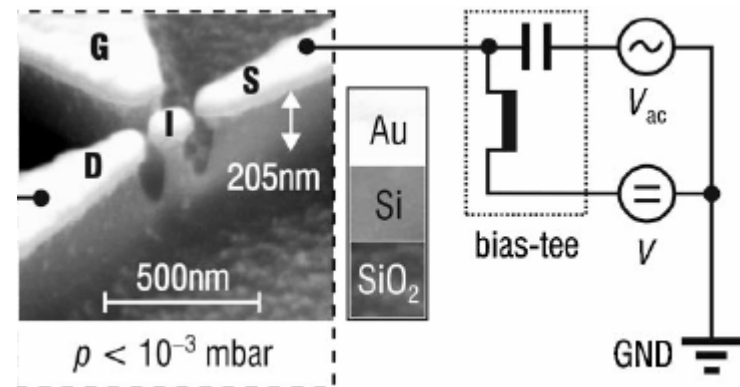
NEM-SET with center-of-mass motion = Mobile Kondo Impurity

Molecular Transistor



H.Park et al, Nature 2000

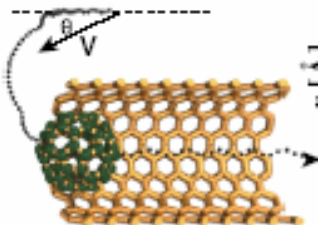
Nano-Pendulum



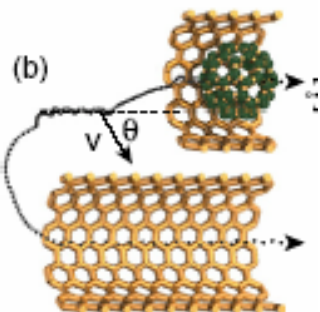
D.Sheible and R.Blick 2004

Nanotube peapods: C_{60} @ CNT

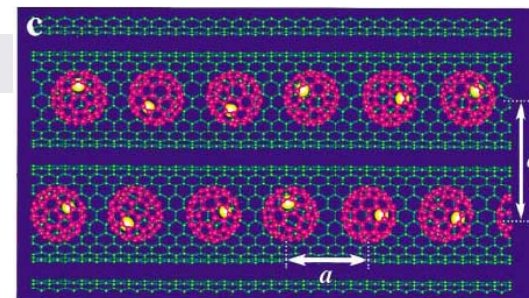
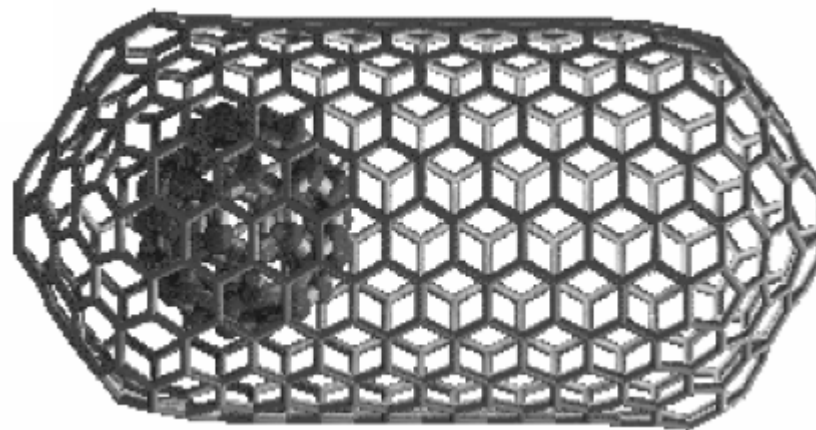
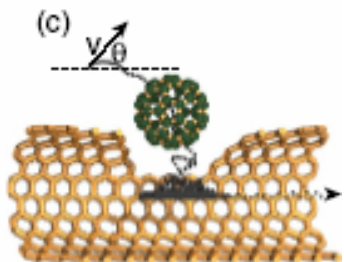
(a)



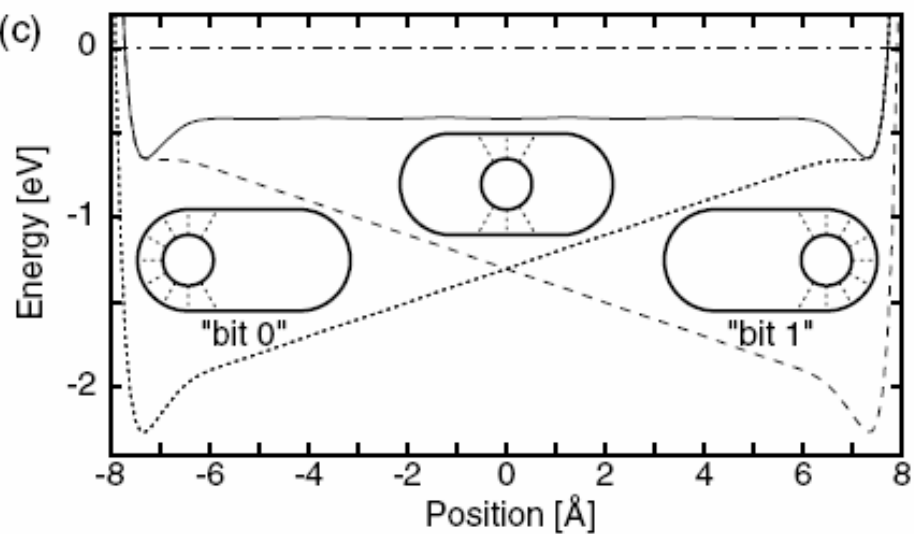
(b)



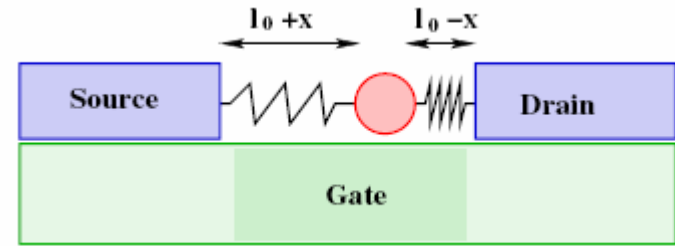
(c)



(c)

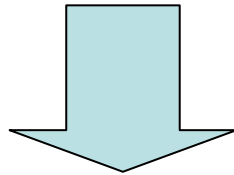


The model



$$H_0 = \sum_{k,\alpha} \varepsilon_{k\sigma,\alpha} c_{k\sigma,\alpha}^\dagger c_{k\sigma,\alpha} + \sum_{i\sigma} [\varepsilon_i - e\mathcal{E}x] d_{i\sigma}^\dagger d_{i\sigma} + Un^2$$

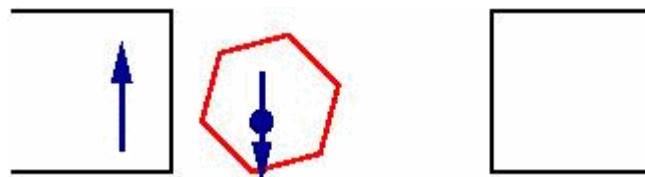
$$H_{tun} = \sum_{ik\sigma,\alpha} [V_\alpha^{(i)}(x) c_{k\sigma,\alpha}^\dagger d_{i\sigma} + H.c],$$



SW transformation

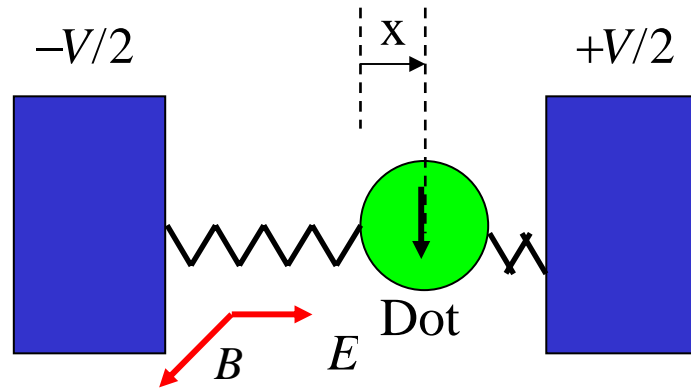
$$H = H_0 + \sum_{k\alpha\sigma, k'\alpha'\sigma'} \mathcal{J}_{\alpha\alpha'}(t) [\vec{\sigma}_{\sigma\sigma'} \cdot \vec{S} + \frac{1}{4} \delta_{\sigma\sigma'}] c_{k\sigma,\alpha}^\dagger c_{k'\sigma',\alpha'}$$

$$\mathcal{J}_{\alpha,\alpha'}(t) = \sqrt{\Gamma_\alpha(t)\Gamma_{\alpha'}(t)} / (\pi\rho_0 E_d(t)) \quad \Gamma_\alpha(t) = 2\pi\rho_0 |V_\alpha(x(t))|^2$$





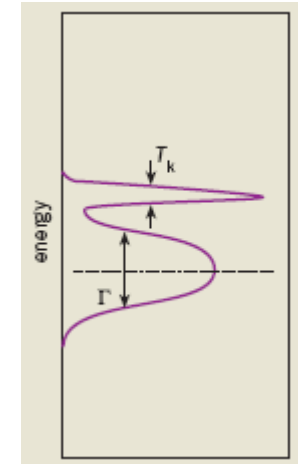
Odd-spin Kondo shuttle



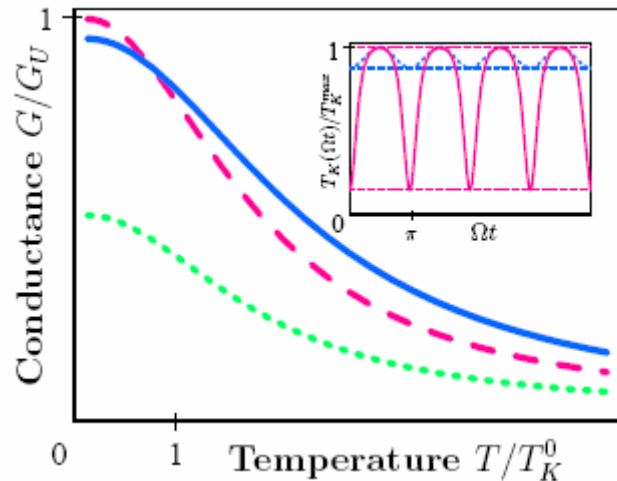
Competition between

Breit-Wigner Resonance

$$G = \frac{2e^2}{h} \left\langle \frac{4\Gamma_L(t)\Gamma_R(t)}{(\Gamma_L(t)+\Gamma_R(t))^2} \right\rangle$$



Abrikosov-Suhl Resonance



$$G(T) = \frac{3\pi^2}{16} G_U \left\langle \frac{4\Gamma_L(t)\Gamma_R(t)}{(\Gamma_L(t)+\Gamma_R(t))^2} \frac{1}{[\ln(T/T_K(t))]^2} \right\rangle$$

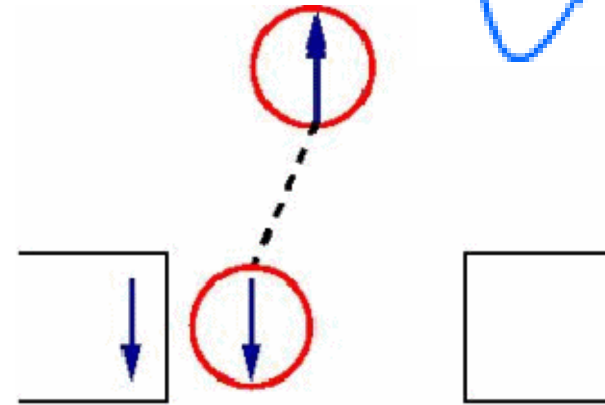
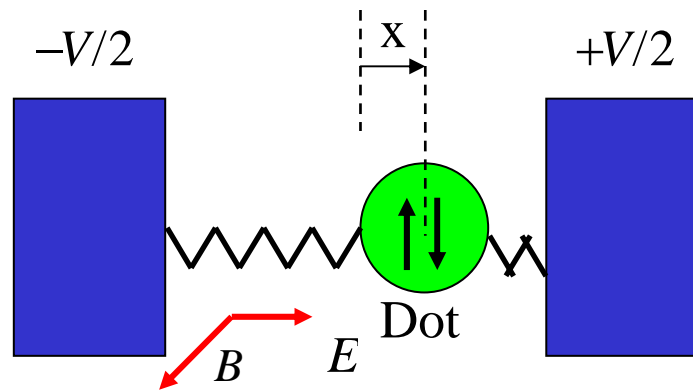
$$T_K(t) = D(t) \exp \left[-\frac{\pi U}{8\Gamma_0 \cosh(2x(t)/\lambda_0)} \right]$$

$$\langle T_K \rangle = T_K^0 \left\langle \exp \left[\frac{\pi U}{4\Gamma_0} \frac{\sinh^2(x(t)/\lambda_0)}{1+2\sinh^2(x(t)/\lambda_0)} \right] \right\rangle$$

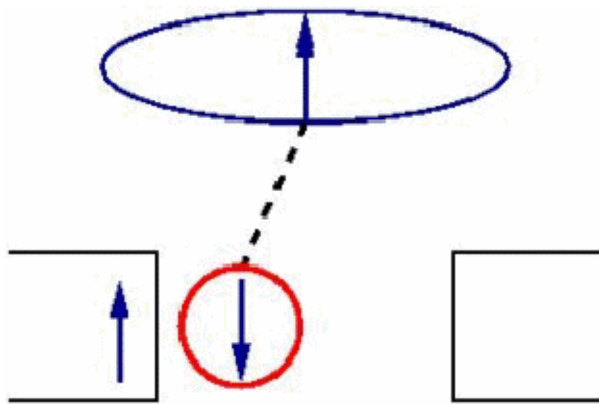
Adiabaticity $\hbar\Omega \ll T_K \ll \Gamma$

Time-dependent Kondo temperatures

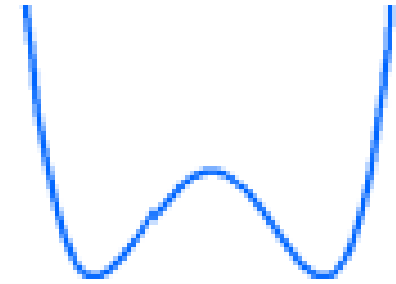
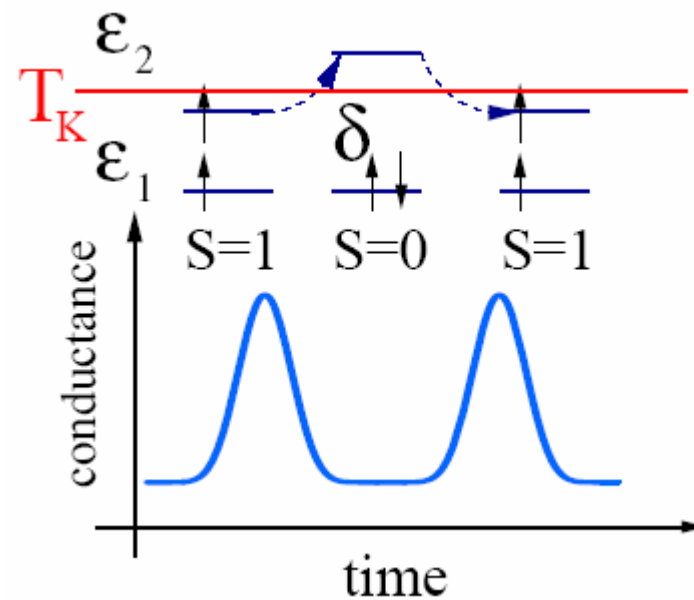
Even-spin Kondo shuttle



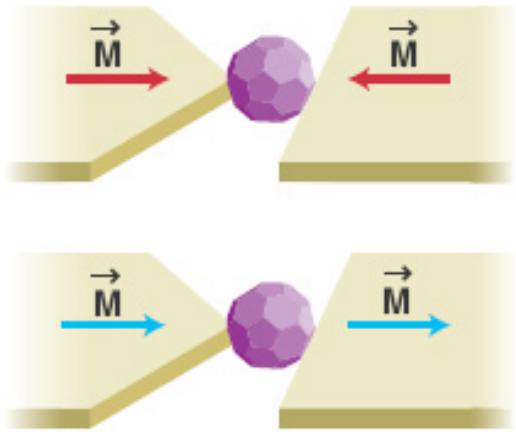
Singlet shuttling: No Kondo effect



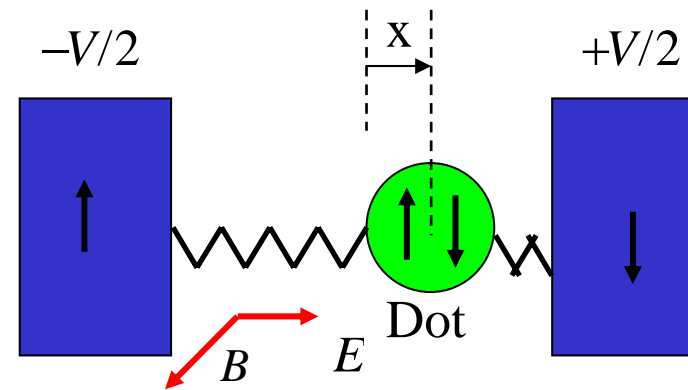
Triplet Kondo Shuttling



Perspectives



A. Pasupathy et al., Science 306,86 (2004)

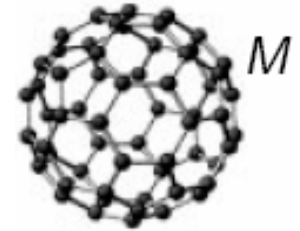


- NEM-SET between spin-polarized leads
- NEM spin manipulation
- Rotating pendulum
- Coupled NEM-SET devices (DQD, TQD)

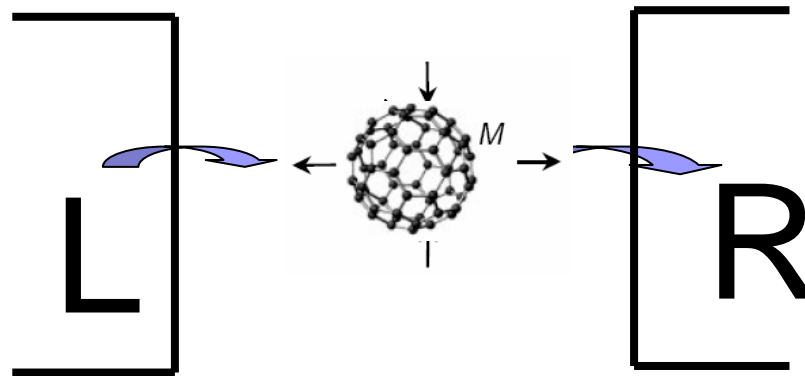


Conclusions

Molecular Transistor



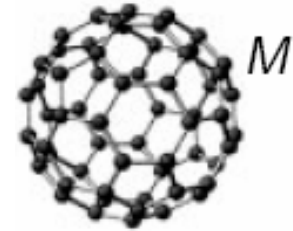
- Phonon emission/absorption induces the Kondo tunneling
- Dynamical symmetries allow Kondo effect in excited triplet state
- Decoherence due to vibration does not destroy the Kondo effect





Conclusions

Molecular Transistor



- Phonon emission/absorption induces the Kondo tunneling
- Dynamical symmetries allow Kondo effect in excited triplet state
- Decoherence due to vibration does not destroy the Kondo effect

Kondo shuttle

- Kondo shuttling allows the spin manipulation by NEM motion
- Kondo NEM-SET is a Mobile Quantum Impurity
- Dynamical symmetries influence the Kondo shuttling in S/T setups