Kondo Shuttling
Single orbital level coupled to two leads

\[ H = H_{\text{leads}} + H_{\text{tun}} + H_{\text{dot}} \]

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

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

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

Tunneling width

\[ \Gamma_{\alpha}(t) = \pi \rho |V_{\alpha}|^2(t) \]
Single orbital level coupled to two leads

Time-dependent Glazman-Raikh rotation

\[
\begin{pmatrix}
c_k \sigma_L \\
c_k \sigma_R
\end{pmatrix} = U_t \begin{pmatrix}
c_k \sigma + \\
c_k \sigma -
\end{pmatrix}
\]

\[U_t = \begin{pmatrix}
\cos \theta_t & -\sin \theta_t \\
\sin \theta_t & \cos \theta_t
\end{pmatrix}\]

\[
\tan \theta_t = \left| \frac{V_R(t)}{V_L(t)} \right|
\]

\[|V|^2(t) = |V_L|^2(t) + |V_R|^2(t)\]

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

Gauge potential

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

Tomosuke Aono, 2004
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

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

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

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

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

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

M. Büttiker et al, 1994
Adiabatic pumping at the Kondo regime

Nozieres Fermi Liquid regime

\[ \delta \sigma \rightarrow \frac{\pi}{2} \]

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

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

Nano-Pendulum

H. Park et al, Nature 2000

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-devise is nano-machined by external periodic force

K. K. Kikoin, MK and M. R. Wegewijs, PRL 2006
MK, K. Kikoin, R. Shekhter and V. Vinokur, PRB 2006
Ferrocene

\[ \text{Fe}(\text{C}_5\text{H}_5)_2 \]
Cerocene \( Ce(C_8H_8)_2 \)

\[ Ce(COT)_2 \]

COT = C8H8
Ytterbocene

$\text{Cp}^*_{2}\text{Yb}\text{(bipy)}$

$\text{Cp}^* = \text{C}5\text{Me}5,$ \quad \text{bipy} = (\text{NC}5\text{H}4)2$
Fullerenes

H.Park et al, Nature 2000
Transition metals inside fullerens
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

\[ H = H_{mol} + H_{res} + H_{tun} \]

\[ H_{mol} = \Pi_Q^{(N)} + \Pi_Q^{(N+1)} + \Pi_Q^{(N-1)} + T_n \]

\[ H_{res} + H_{tun} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \tilde{\omega}_Q \sum_{k\mu\sigma} \left( \tilde{d}_{\mu\sigma}^\dagger c_{k\sigma} + H.c. \right) \]
cage MO = localized

dipolar

e- M+ M- e-

cage MO = delocalized

quadrupolar

e- M+ M- e-

breathing

e-

\[ \Delta \equiv E_T - E_S = \delta - I > T_K \]

Triplet  Singlet  Exchange
**TMOC = Transition Metal + Organic Complex (cage)**

\[
H_{mol}^{(N)} = \sum_{\Lambda=S,T0,T\pm} E_{\Lambda}(Q)|\Lambda\rangle\langle\Lambda|
\]

Assumption: even electron occupation number

Singlet is a ground state

SO(4) symmetry

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

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

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

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

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

\[ \hat{J}_{S,R} \]

\[ \hat{j}_R \]

\[ \hat{j}_S \]

\[ S \quad T \quad T \quad T \]

single phonon \hspace{1cm} \text{two-phonon}

\[ j_S \ll j_R \]
Phonon assisted processes

single-phonon

t_1 \quad t_n

t_i \quad t_f

t_1 \quad t_n

t_i \quad t_f

two-phonon
Single phonon processes

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

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

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

Summation of “parquet” diagrams

$$\gamma_1 \sim j_R^2 \int \frac{d\epsilon}{2\pi} \coth \left( \frac{\epsilon}{2T} \right) \left[ \text{Re} \left[ \frac{\Pi(\epsilon)}{1 - J_T^T \bar{\Pi}(-\epsilon)} \right]^R \text{Im} D^R(\epsilon) + \text{Re} D^R(-\epsilon) \text{Im} \left[ \frac{\Pi_1(\epsilon)}{1 - J_T^T \bar{\Pi}(\epsilon)} \right]^R \right]$$
Single phonon processes

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

\[ 1 - J_S A \rho \log \left( \frac{D}{\max[T, |\Delta - \Omega|]} \right) \]

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

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

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

\[ \frac{dI}{dV} \]

Strong decoherence regimes

Non-equilibrium Kondo (S/T transitions)

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

Equilibrium Kondo temperature (triplet state)

S/T splitting

\[ |\Delta - \Omega_0| \]
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

S=1 Kondo effect → S=1/2 Kondo effect

M.Pustilnik, Y.Avishai, K.Kikoin, PRL 2000
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

Nano-Pendulum

H. Park et al, Nature 2000

D. Sheible and R. Blick 2004
Nanotube peapods: \( C_{60} @ CNT \)
The model

\[ H_0 = \sum_{k,\alpha} \varepsilon_{k\sigma,\alpha} c_{k\sigma,\alpha}^{\dagger} c_{k\sigma,\alpha} + \sum_{i\sigma} [\epsilon_i - eE x] d_{i\sigma}^{\dagger} d_{i\sigma} + U n^2 \]

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

**SW transformation**

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

\[ \mathcal{J}_{\alpha,\alpha'}(t) = \sqrt{\Gamma_{\alpha}(t)\Gamma_{\alpha'}(t)/(\pi \rho_0 E_d(t))} \quad \Gamma_{\alpha}(t) = 2\pi \rho_0 |V_{\alpha}(x(t))|^2 \]
Odd-spin Kondo shuttle

Competition between

Breit-Wigner Resonance

\[ G = \frac{2e^2}{\hbar} \left< \frac{4\Gamma_L(t)\Gamma_R(t)}{(\Gamma_L(t) + \Gamma_R(t))^2} \right> \]

Abrikosov-Suhl Resonance

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

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

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

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

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


B: magnetic field
E: electric field
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