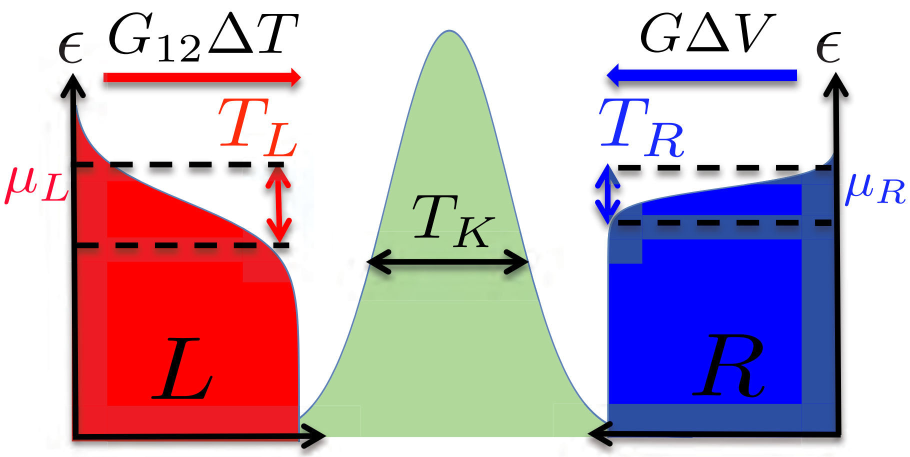
The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

M.N.Kiselev

Thermoelectrics transport through SU(N) Quantum Impurity

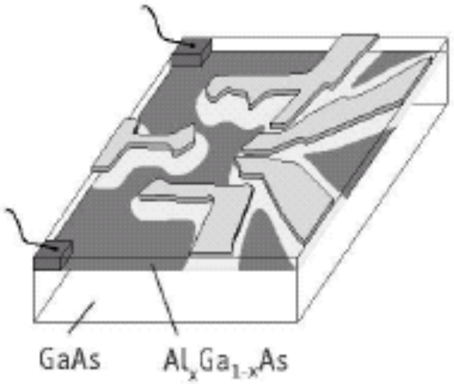


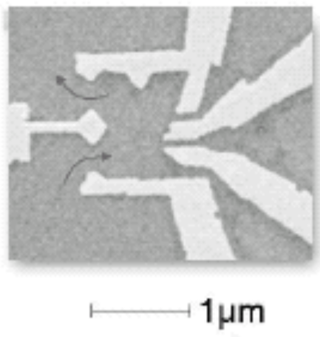
ICTP, March 14, 2019

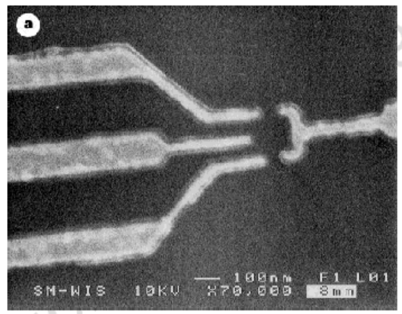
D.B. Karki and MK, PRB **96**, 121403(R) (2017)

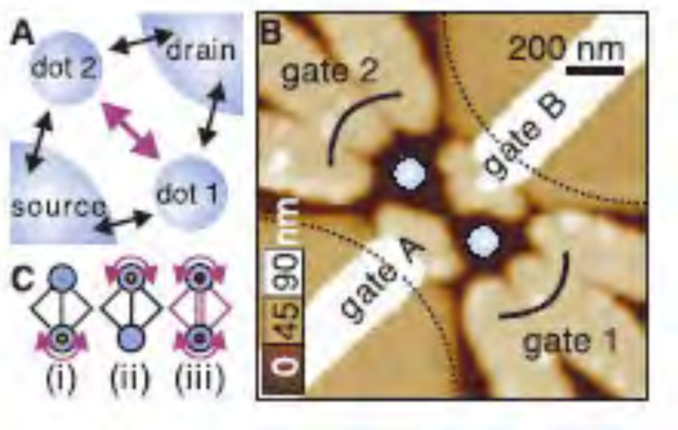
T. K. T. Nguyen and MK, PRB 97, 085403 (2018)

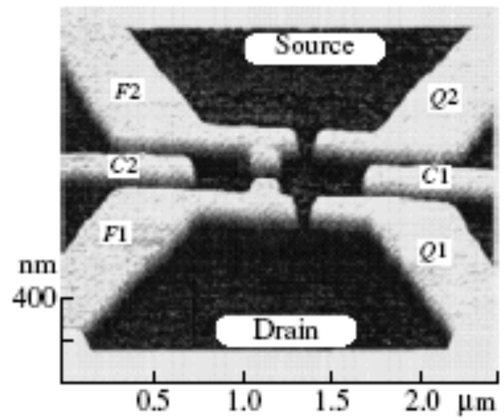
Quantum dots: from simple to complex

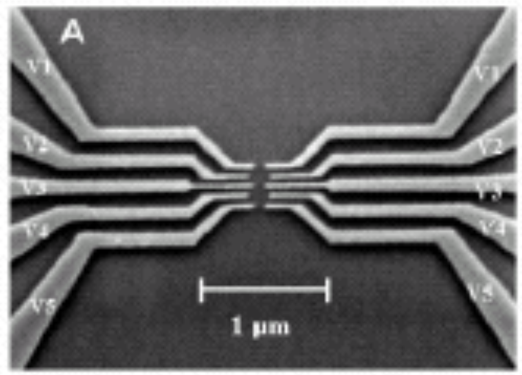












D. Goldhaber-Gordon et al (1998)

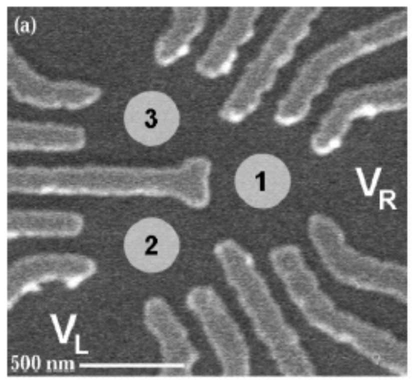
J.P. Kotthaus (1995)

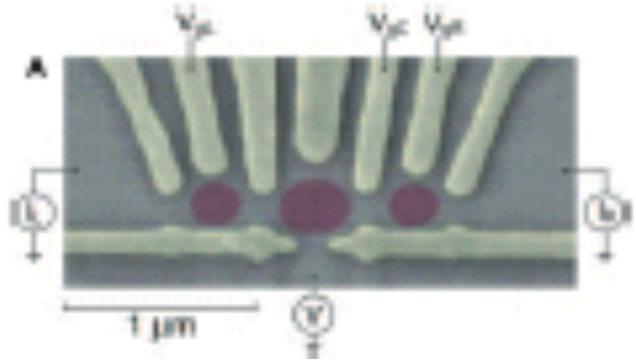
A. Holleitner et al (2002)

L.W. Molenkamp et al (1995)

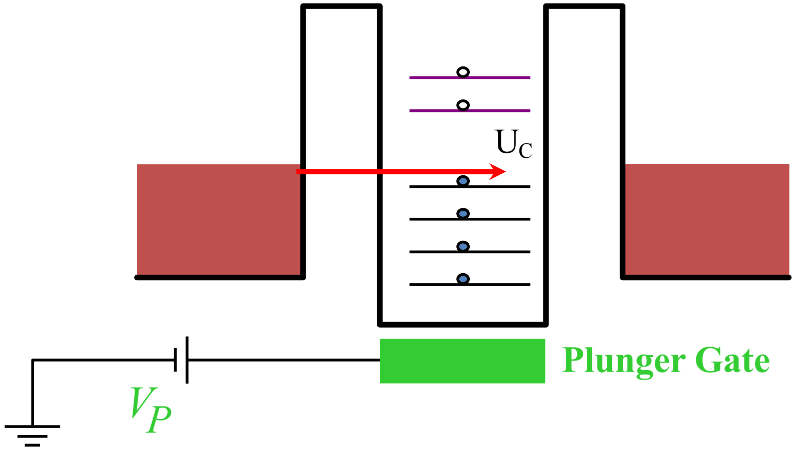
H. Jeong et al (2001)

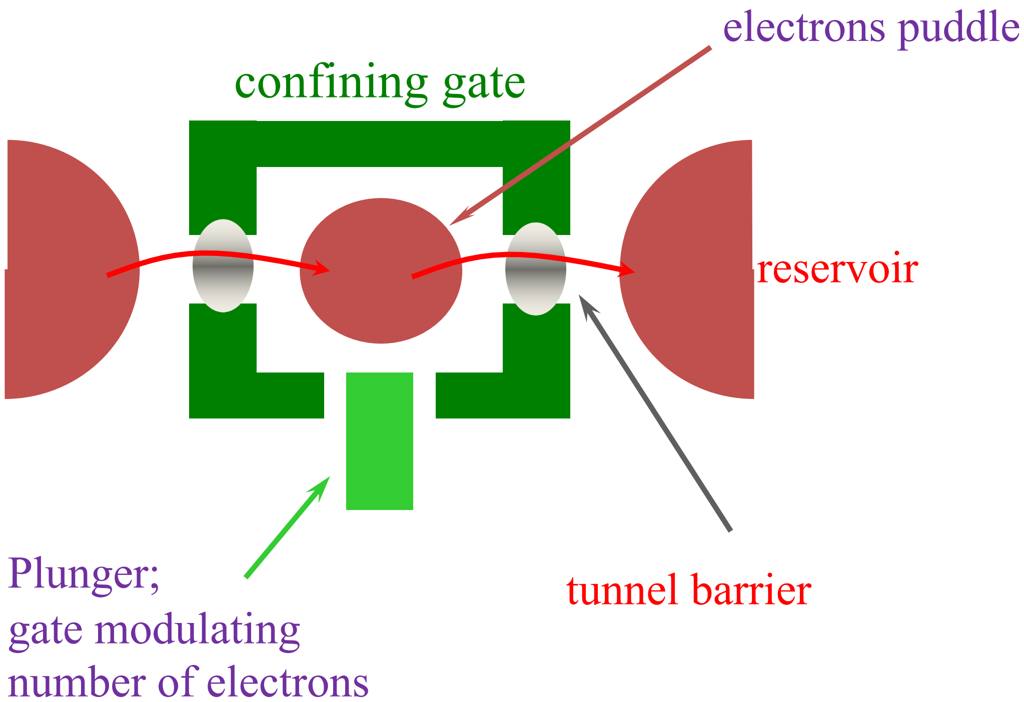
C. Marcus et al (2003)

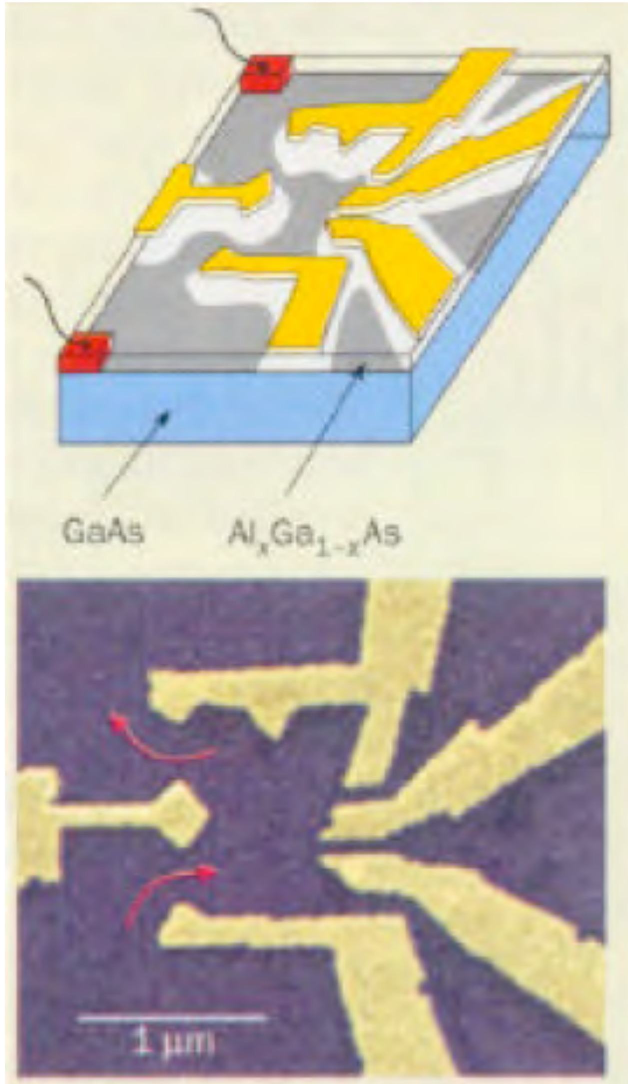




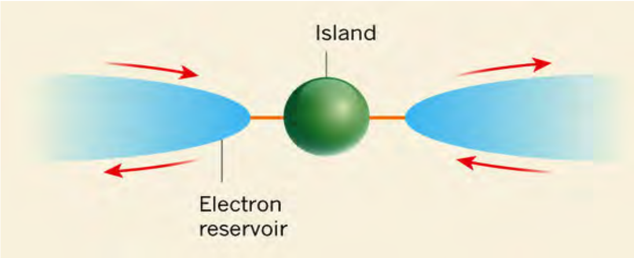
Realization of lateral QD in 2DEG



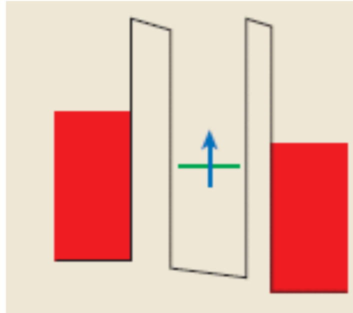




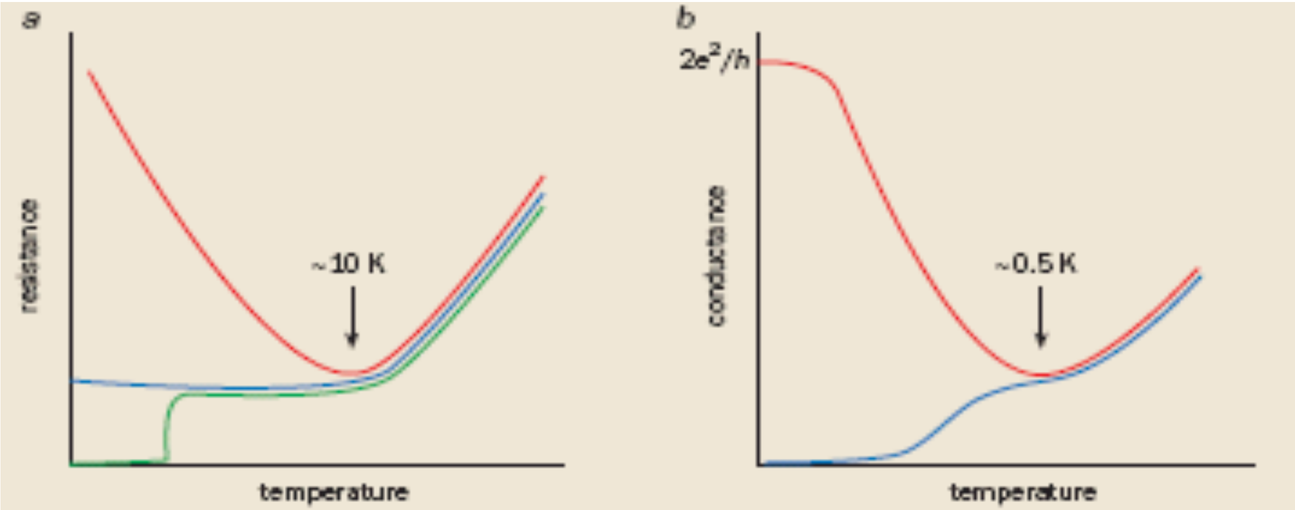
Quantum Impurity: Kondo Effect



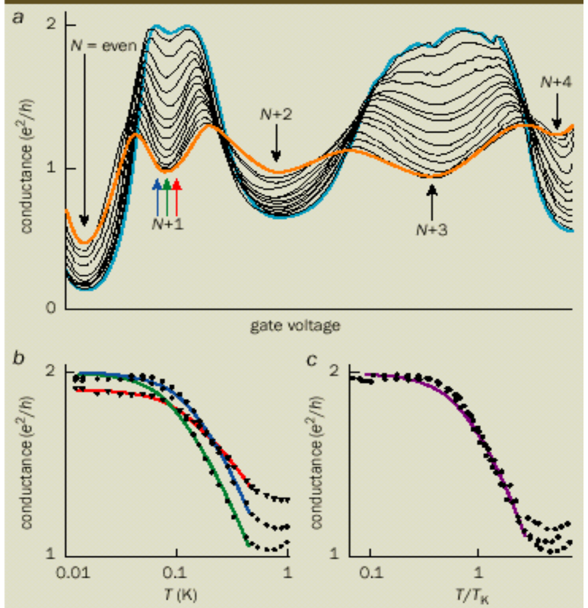
$$H_K = J\,\vec{s}\cdot\vec{S}$$



$$H = \sum_{k\alpha\sigma} \xi_k c^\dagger_{\alpha k\sigma} c_{\alpha k\sigma} + \sum_{\sigma} \epsilon_0 d^\dagger_\sigma d_\sigma + \sum_{\sigma\neq\sigma'} U d^\dagger_\sigma d_\sigma d^\dagger_{\sigma'} d_{\sigma'} + \sum_{k\alpha\sigma} t_\alpha d^\dagger_\sigma c_{\alpha k\sigma} + c.c.$$



5 Universal scaling



(a) The conductance (y-axis) as a function of the gate voltage, which changes the number of electrons, N, confined in a quantum dot. When an even number of electrons is trapped, the conductance decreases as the temperature is lowered from 1 K (orange) to 25 mK (light blue). This behaviour illustrates that there is no Kondo effect when N is even. The opposite temperature dependence is observed for an odd number of electrons, i.e. when there is a Kondo effect. (b) The conductance for $N + 1$ electrons at three different fixed gate voltages indicated by the coloured arrows in (a). The Kondo temperature, T_K, for the different gate voltages can be calculated by fitting the theory to the data. (c) When the same data are replotted as a function of temperature divided by the respective Kondo temperature, the different curves lie on top of each other, illustrating that electronic transport in the Kondo regime is described by a universal function that depends only on T/T_K.

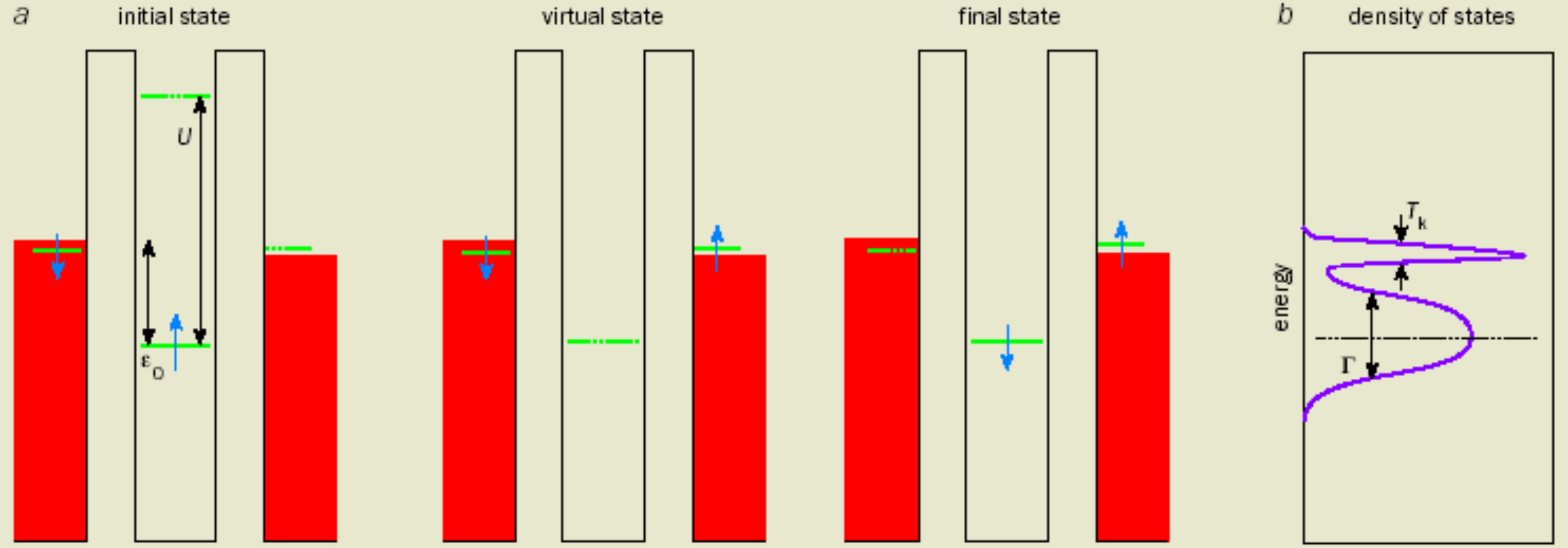
$$G/G_0 \propto \ln^{-2}\left(\max[T/T_K]\right)$$

$$T_K = \frac{1}{2}(\Gamma U)^{1/2}\exp\left(\pi\varepsilon_0\frac{\varepsilon_0+U}{\Gamma U}\right) \qquad \Gamma = \pi|t|^2\nu(\varepsilon_F)$$

Kondo Effect in Quantum Dots

$$H_K = \sum_{k\alpha\sigma,k'\alpha'\sigma'} J_{\alpha\alpha'}[\vec{\sigma}_{\sigma\sigma'}\vec{S} + \frac{1}{4}\delta_{\sigma\sigma'}]c^{\dagger}_{k\sigma,\alpha}c_{k'\sigma',\alpha'}$$

2 Spin flips



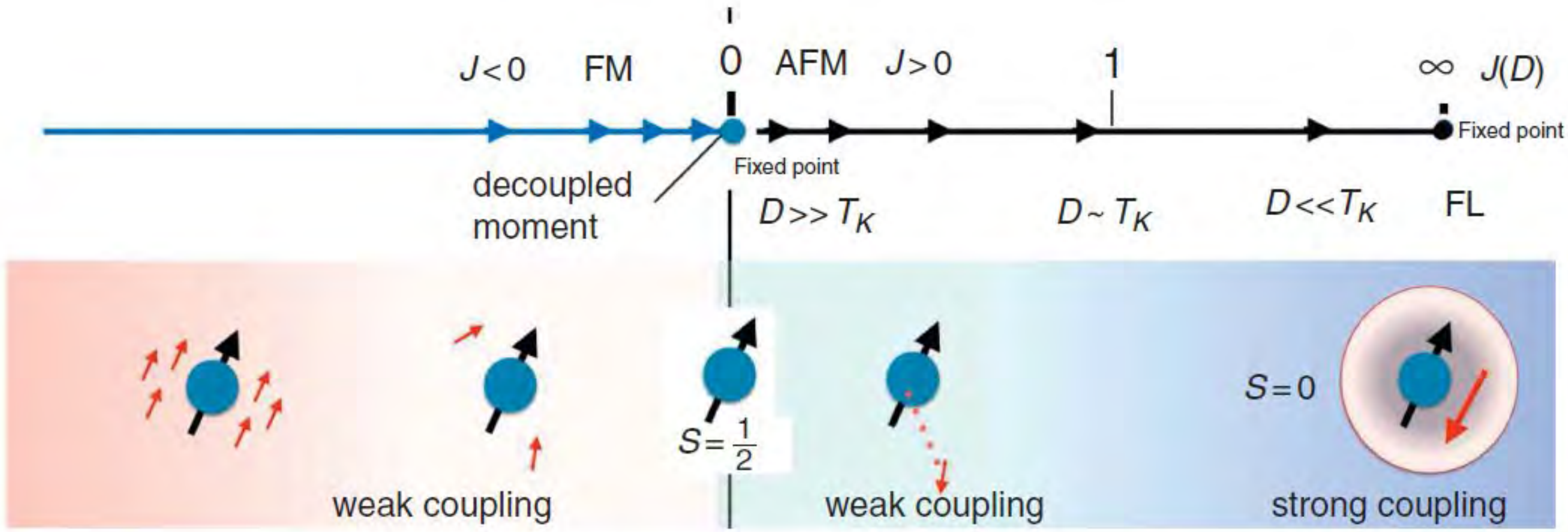
(a) The Anderson model of a magnetic impurity assumes that it has just one electron level with energy ε_0 below the Fermi energy of the metal (red). This level is occupied by one spin-up electron (blue). Adding another electron is prohibited by the Coulomb energy, U, while it would cost at least $|\varepsilon_0|$ to remove the electron. Being a quantum particle, the spin-up electron may tunnel out of the impurity site to briefly occupy a classically forbidden "virtual state" outside the impurity, and then be replaced by an electron from the metal. This can effectively "flip" the spin of the impurity. (b) Many such events combine to produce the Kondo effect, which leads to the appearance of an extra resonance at the Fermi energy. Since transport properties, such as conductance, are determined by electrons with energies close to the Fermi level, the extra resonance can dramatically change the conductance.

Kondo model

$$H_K = \sum_{k\alpha\sigma,k'\alpha'\sigma'} J_{\alpha\alpha'}[\vec{\sigma}_{\sigma\sigma'}\vec{S} + \frac{1}{4}\delta_{\sigma\sigma'}]c^{\dagger}_{k\sigma,\alpha}c_{k'\sigma',\alpha'}$$

$$J \to \mathcal{J} = \frac{J}{1-\nu J\ln(D/T)}$$ $T \gg T_K$ Weak coupling regime, perturbation theory

$$T_K = D\exp\left(-\frac{1}{\nu J}\right)$$ $T \ll T_K$ Strong coupling regime, non-perturbative

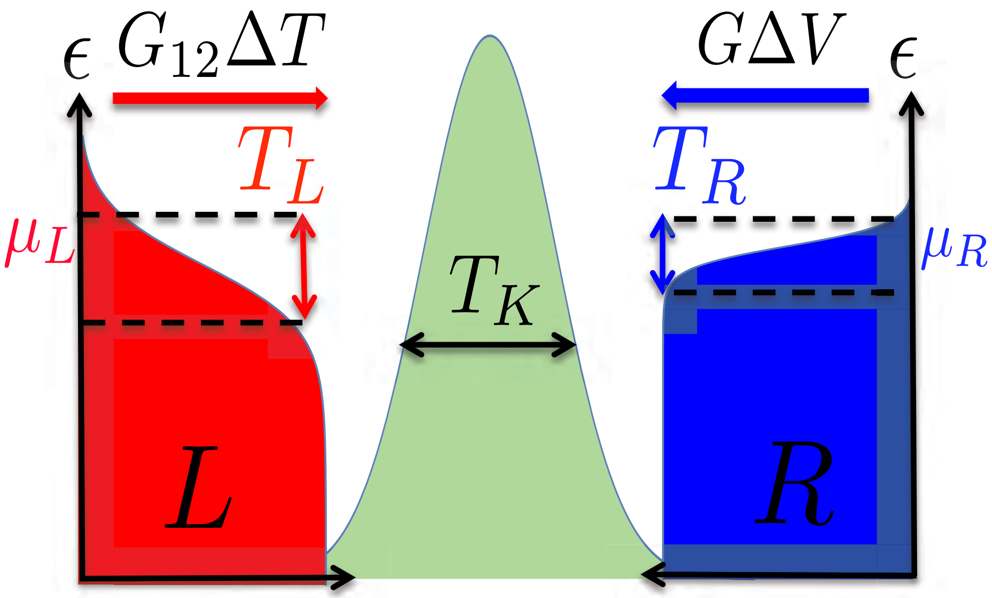


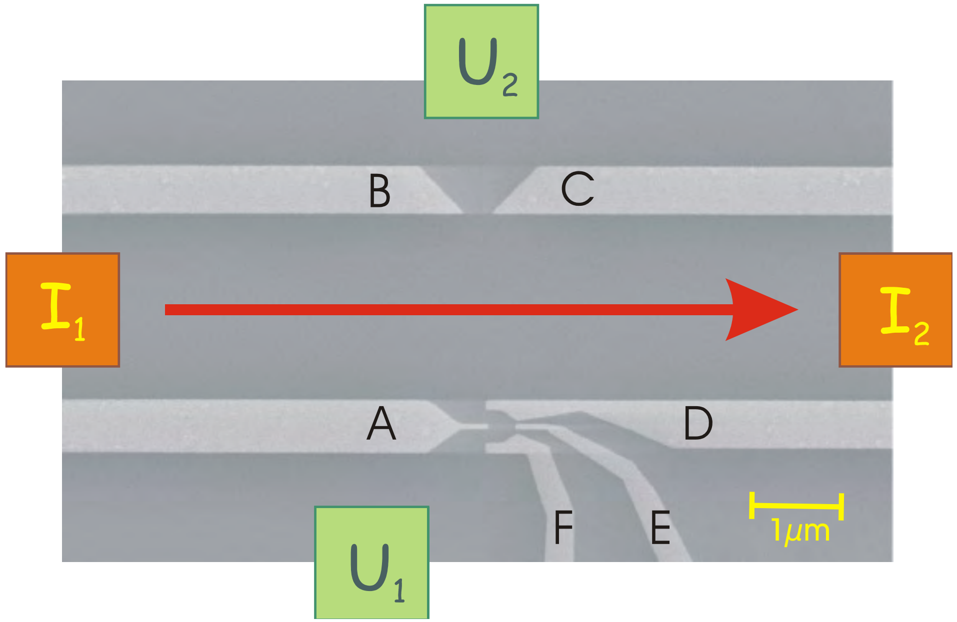
Outline

- Seebeck effect in nanostructures
- Thermoelectrics of SU(2) Kondo impurity
- SU(N): theoretical dreams and experimental realities
- SU(N) Kondo thermoelectrics at strong coupling
- SU(N) : Fermi Liquid vs non-Fermi Liquid
- Messages to take home

Thermoelectric transport through nanostructures (Seebeck effect)

thermopower $$\boxed{S = -\frac{V}{\Delta T}} = \frac{G_{12}}{G}$$





$$I = G \cdot V + G_{12} \cdot \Delta T = 0$$

Thermoelectric transport: FL description

Bulk metals (Fermi Liquid Theory):

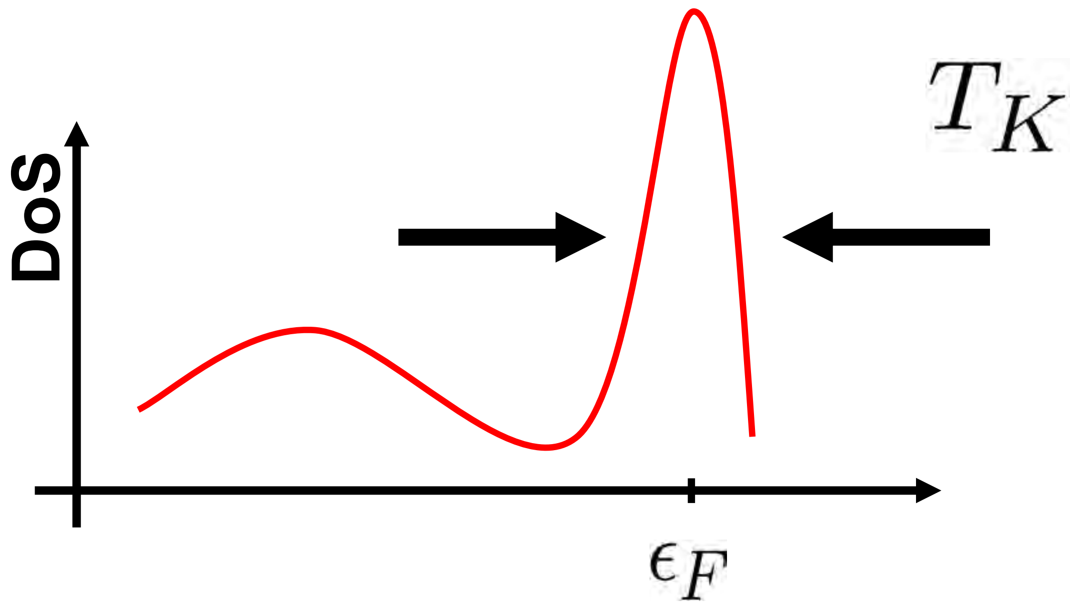
$$S \sim T/\epsilon_F \xrightarrow{\text{strongly correlated metals}} S \sim T/T^*$$

$$T^* \ll \epsilon_F$$

strong electron-electron interaction

resonance scattering effects

Example: Kondo effect

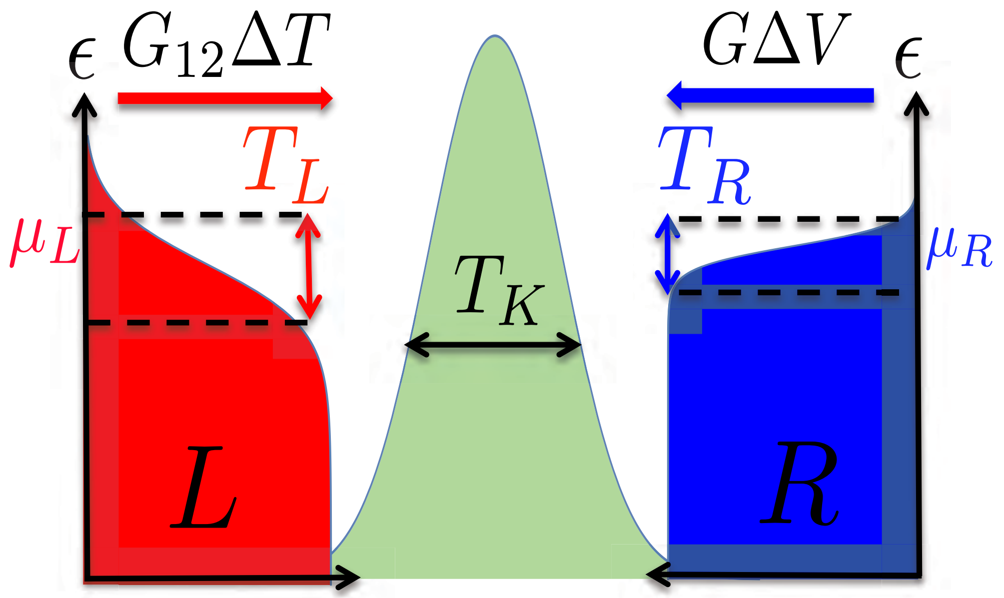


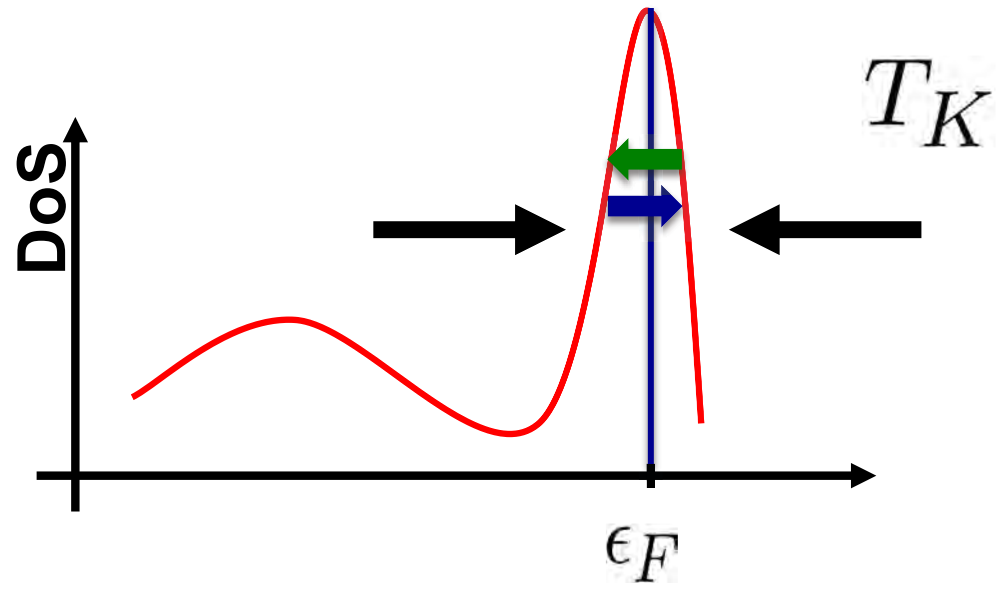
$$S \sim T/T_K$$

Thermoelectric transport: Kondo regime

particle-hole symmetry

$$G_{12} = \left.\frac{\partial I}{\partial \Delta T}\right|_{V=0} = 0 \longrightarrow S = 0$$





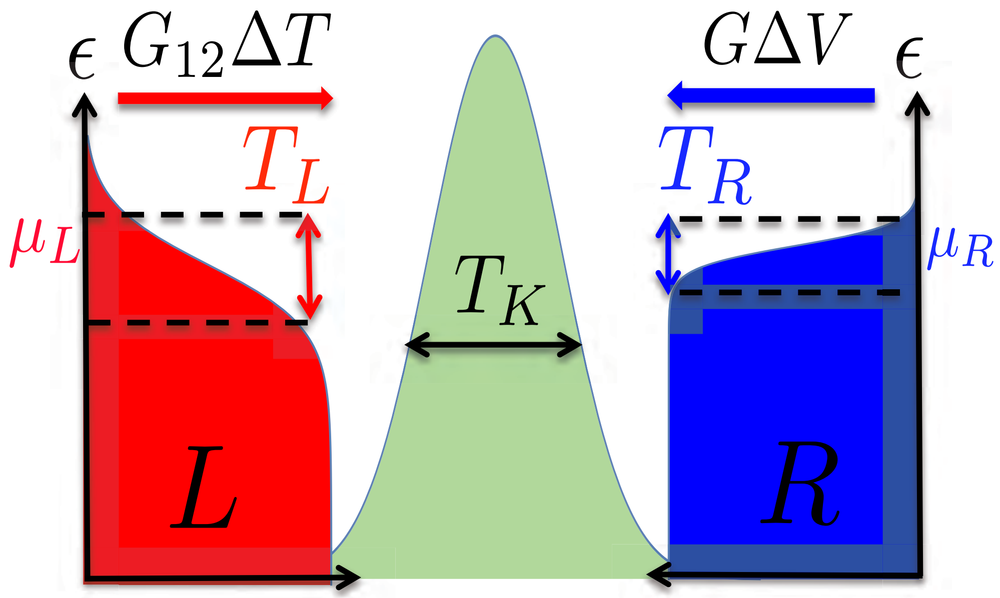
$$I = G \cdot V + G_{12} \cdot \Delta T = 0$$

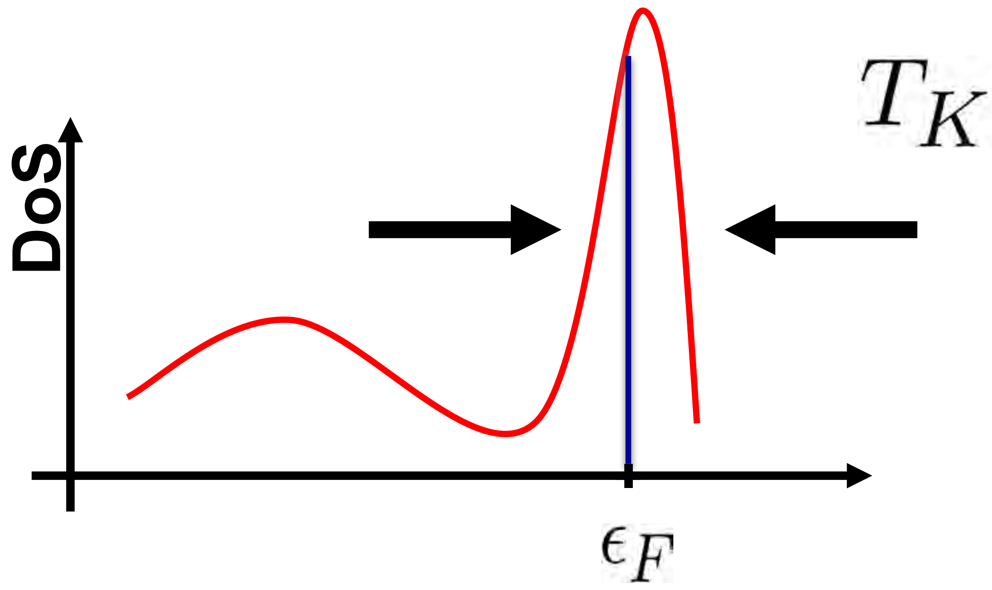
Thermoelectric transport: Kondo regime

breaking the particle-hole symmetry

$$S \sim \frac{\partial \ln G}{\partial V_g}$$

"huge" TP





$$I = G \cdot V + G_{12} \cdot \Delta T = 0$$

Thermoelectric transport through QD

PHYSICAL REVIEW B VOLUME 46, NUMBER 15 15 OCTOBER 1992-I

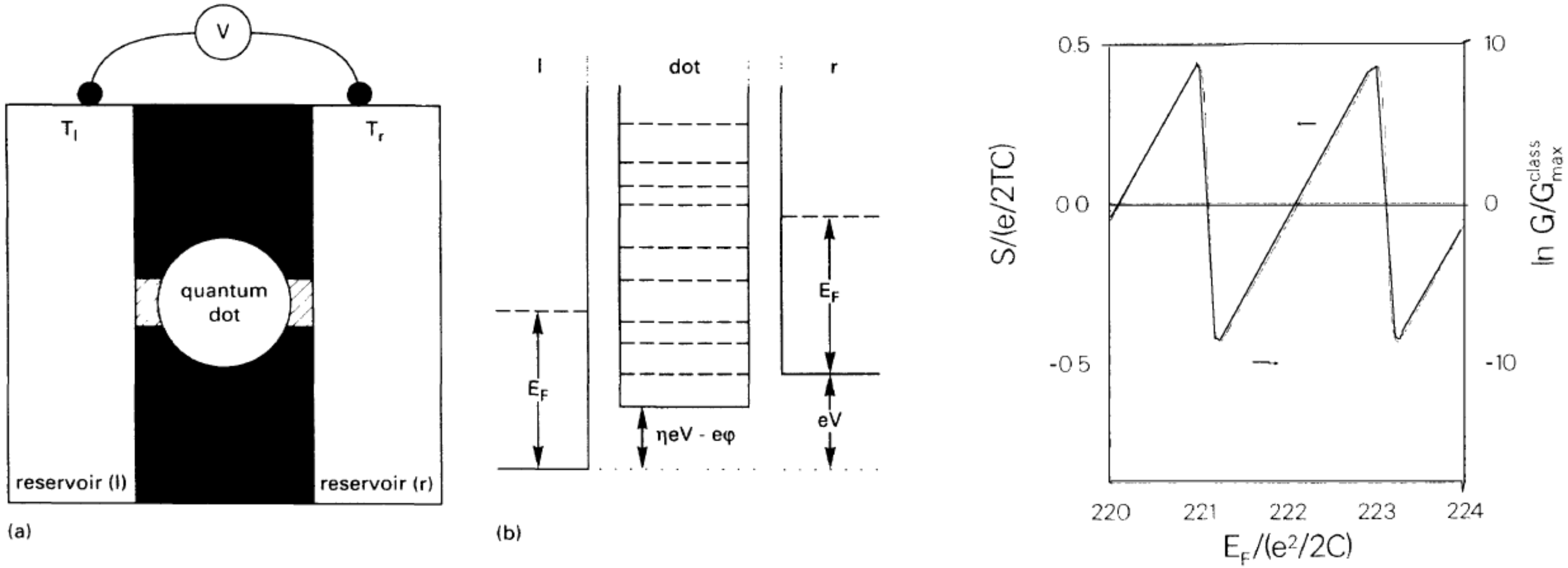
Theory of the thermopower of a quantum dot

C. W. J. Beenakker
Instituut-Lorentz, University of Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

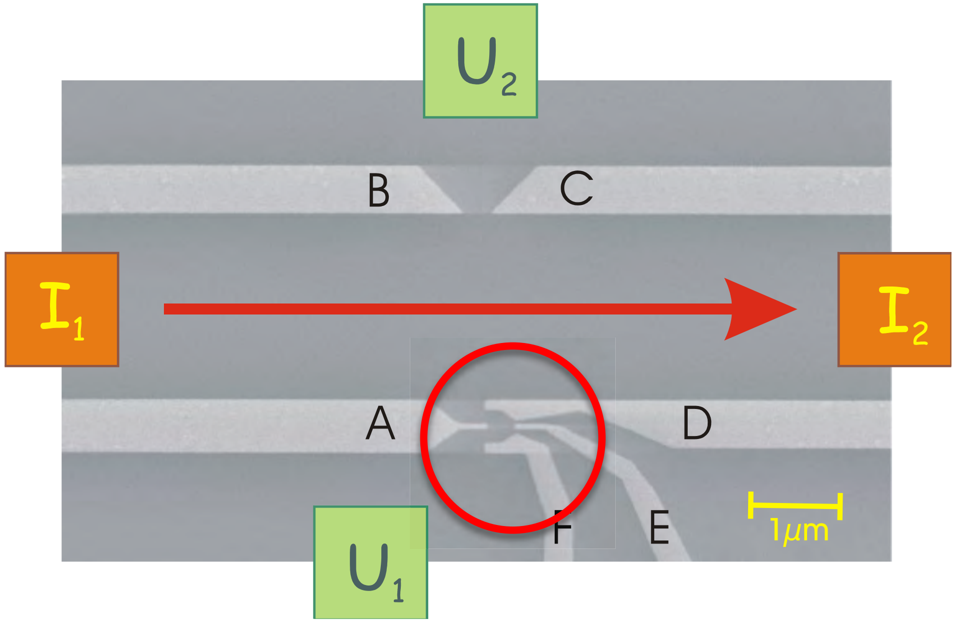
A. A. M. Staring
Philips Research Laboratories, P.O. Box 80000, 5600 JA Eindhoven, The Netherlands

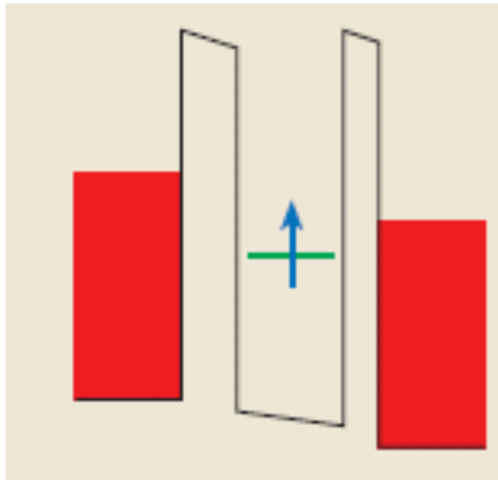
(Received 15 April 1992)

A linear-response theory is presented for the thermopower of a quantum dot of small capacitance. In the *classical* regime (thermal energy kT much greater than the level spacing ΔE), the thermopower oscillates around zero in a sawtooth fashion as a function of Fermi energy (as long as kT is small compared to the charging energy e^2/C). The periodicity of the oscillations is the same as that of the previously studied Coulomb-blockade oscillations in the conductance, and is determined by the difference in ground-state energies on addition of a single electron to the quantum dot. In the *quantum* regime of resonant tunneling ($kT \ll \Delta E$), a fine structure is predicted to develop on the oscillations. Unlike the Coulomb-blockade oscillations, the periodicity of the fine structure is determined by the excitation spectrum at a *constant* number of electrons on the quantum dot.



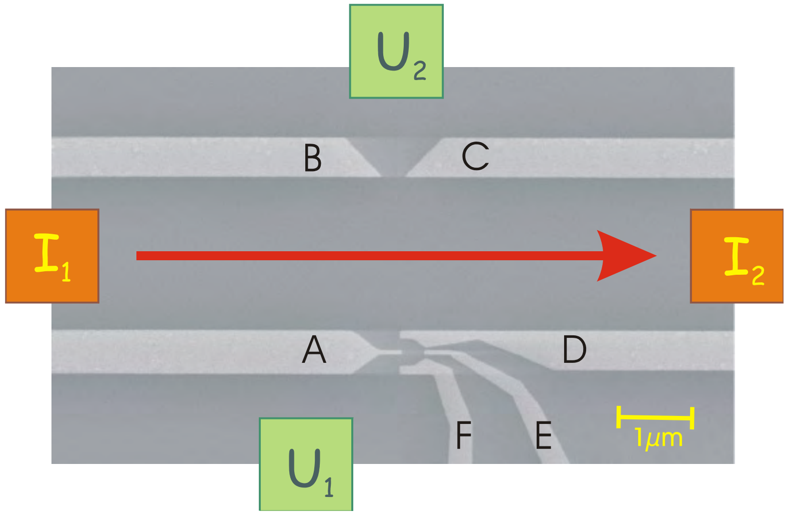
Is there any puzzle for QD in the Kondo regime ?

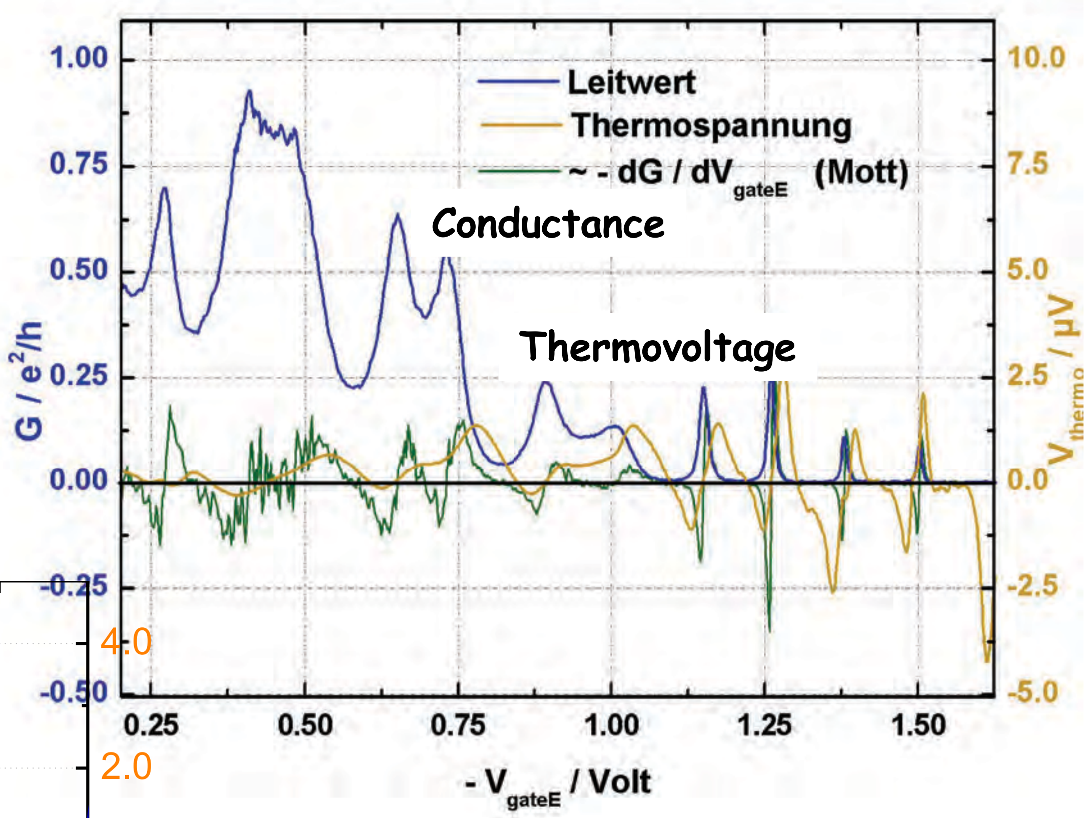


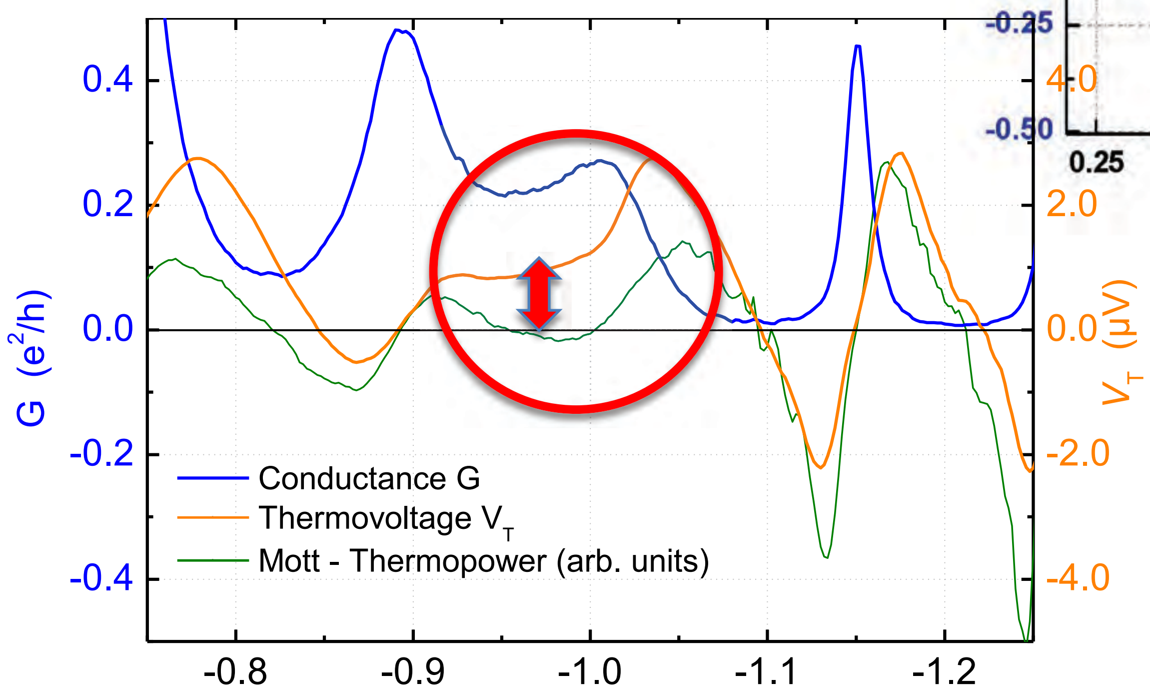


Thermoelectrics of SU(2) Kondo

From weak to strong coupling







$$S \sim \frac{\partial \ln G}{\partial V_g}$$

L.W. Molenkamp, MK et al, PRL 2005

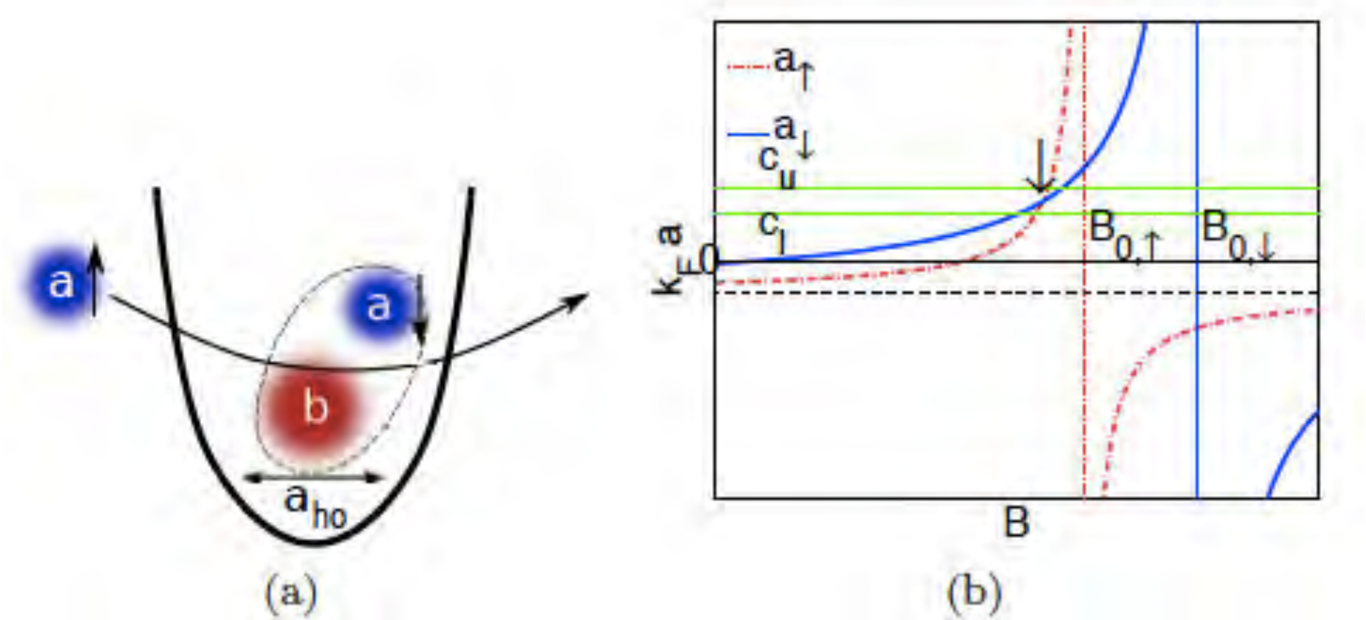
Why to care about the SU(N) ?

What is a challenge ?

Chance to stay away from the particle-hole symmetry
and the same time keep the advantages of Kondo

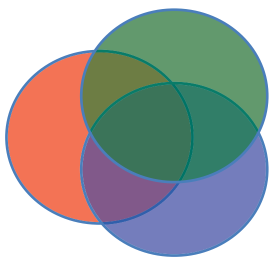
SU(N) Kondo: theoretical suggestions

SU(2) Kondo effect in ultra-cold gases



J. Bauer, C. Salomon and E. Demler, PRL 2013

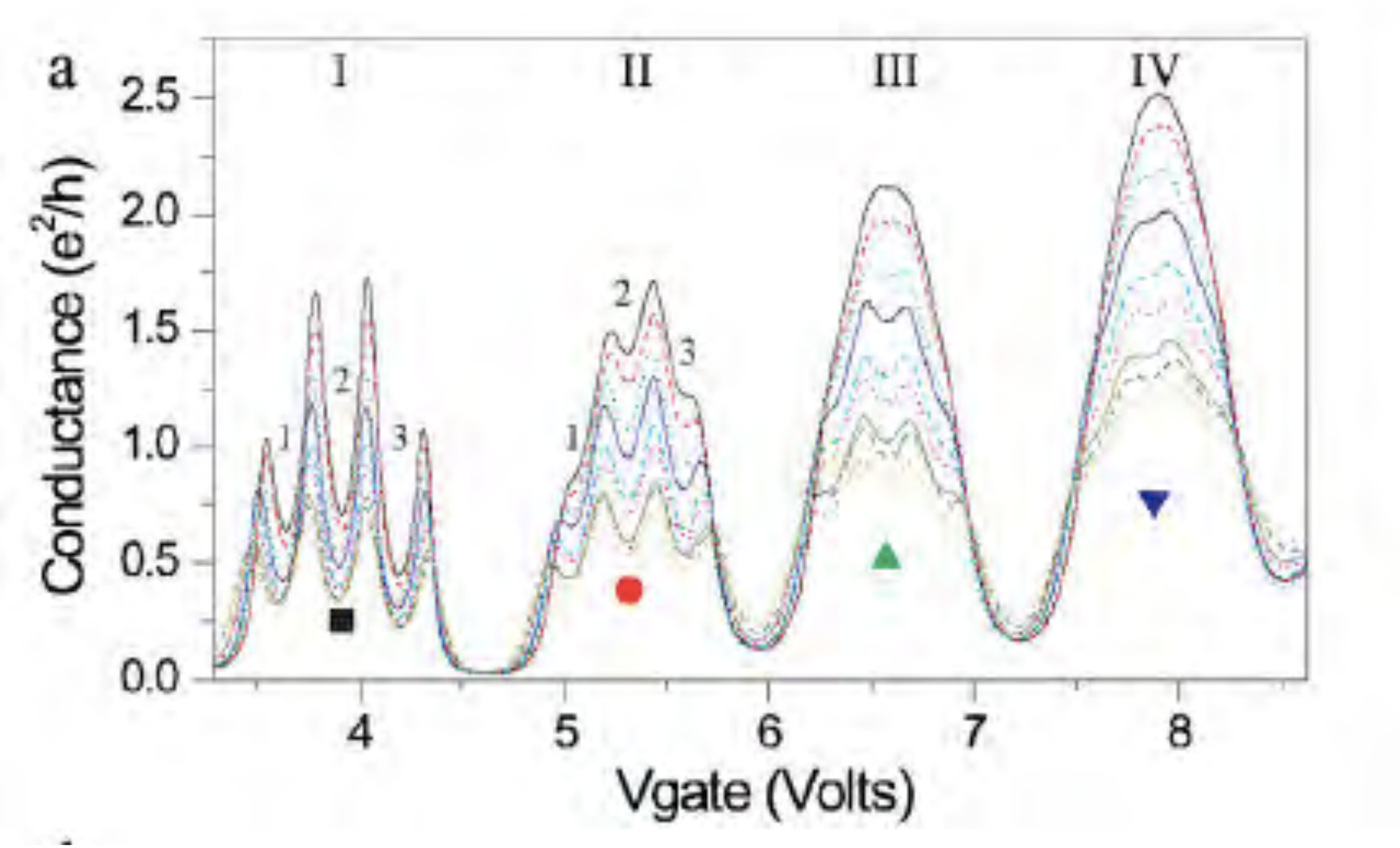
SU(3) Kondo effect in ultra-cold gases



Y. Nishida, PRL 2013, PRB 2015

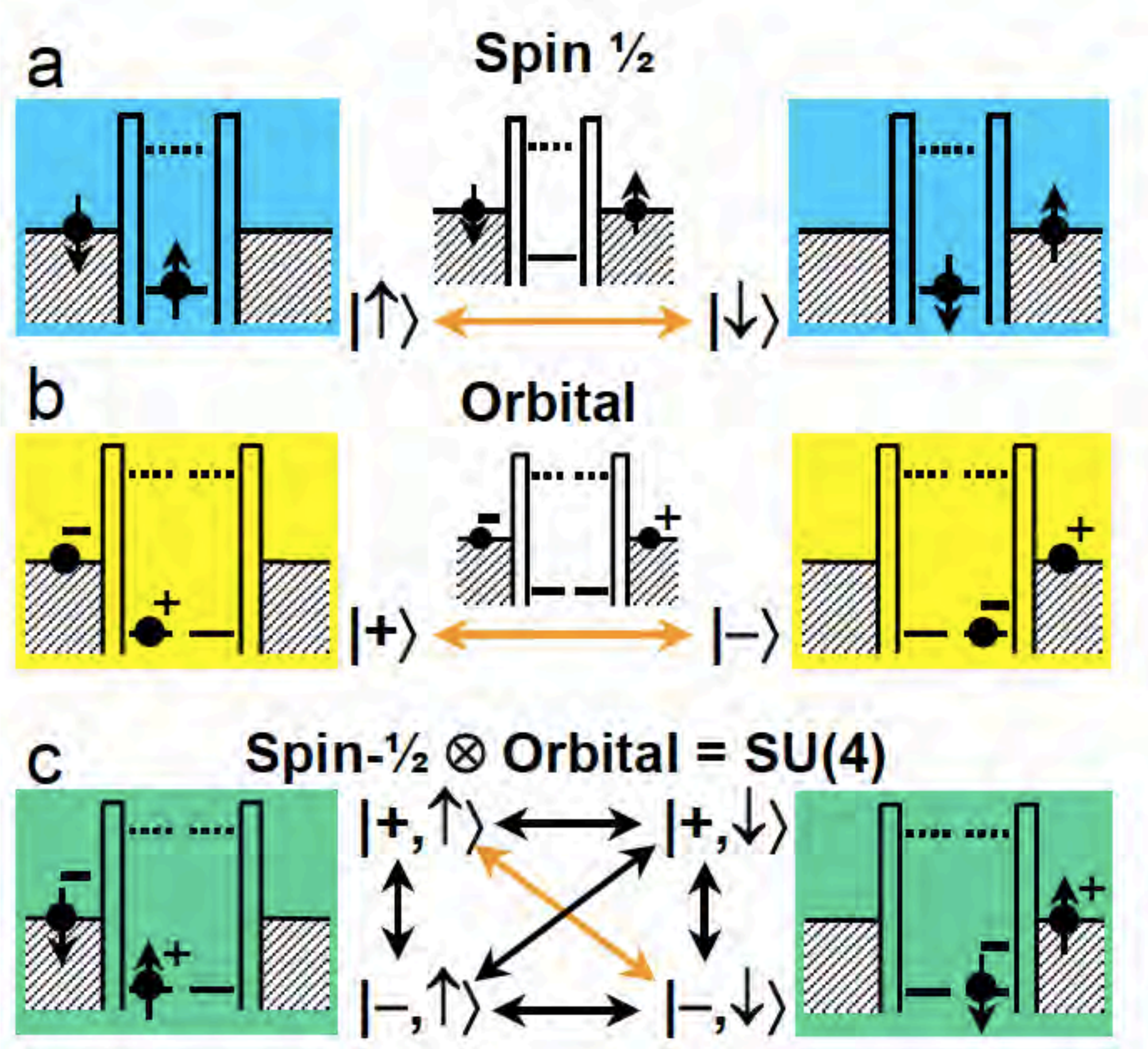
SU(N) Kondo: experimental reality

SU(4) Kondo effect in CNT



A. Marakovski et al PRL and PRB 2007

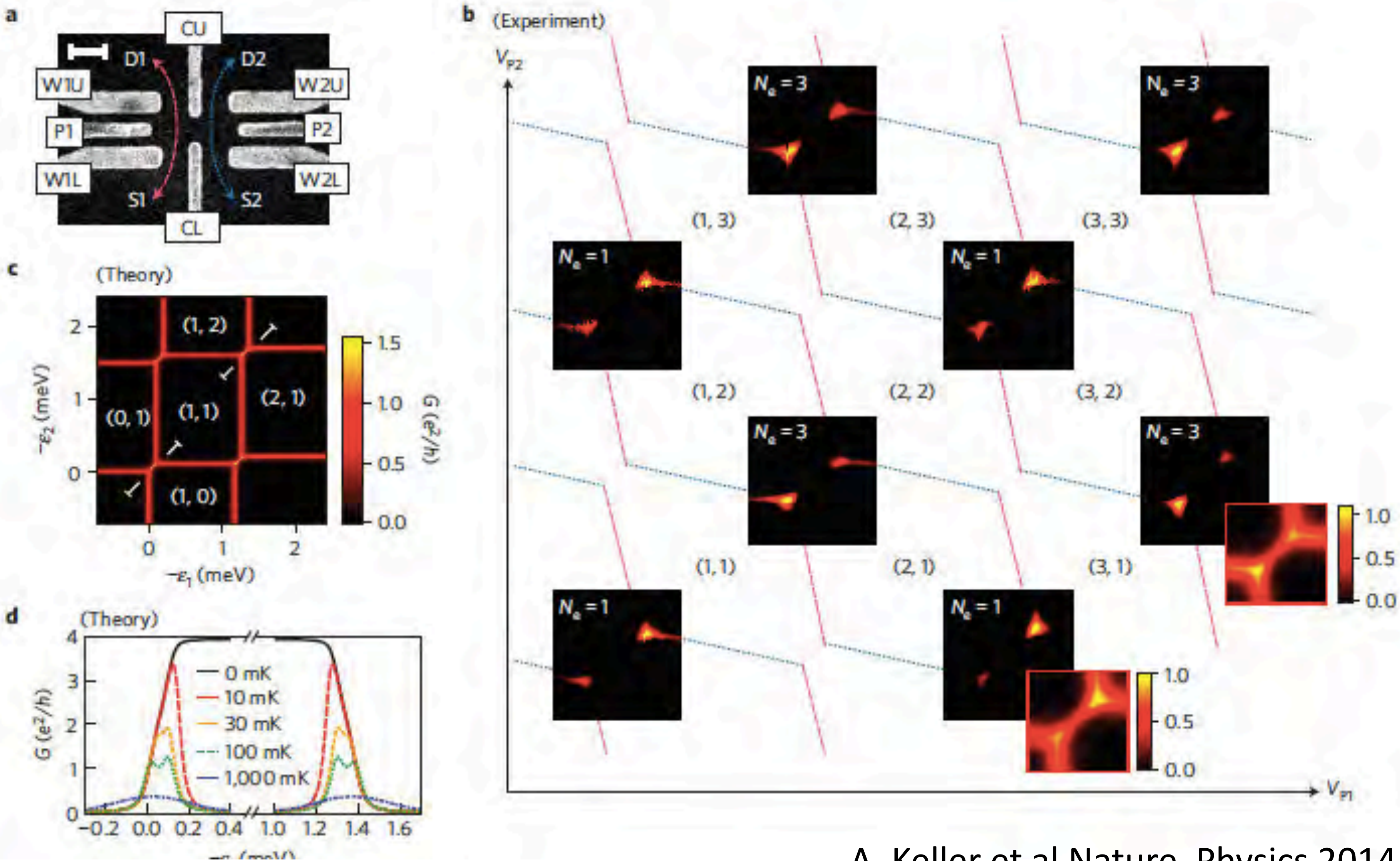
SU(4) Kondo effect in CNT



P. Jarillo-Herrero et al, Nature 2005

SU(N) Kondo: experimental reality

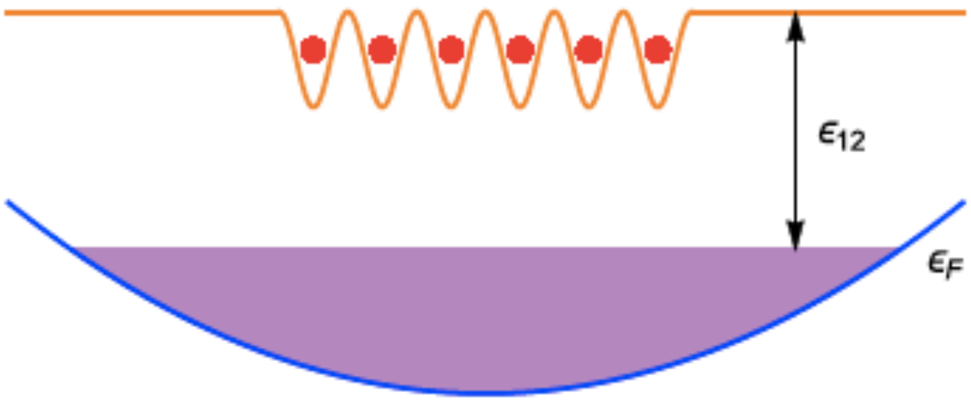
SU(4) Kondo effect in DQD



A. Keller et al Nature Physics 2014

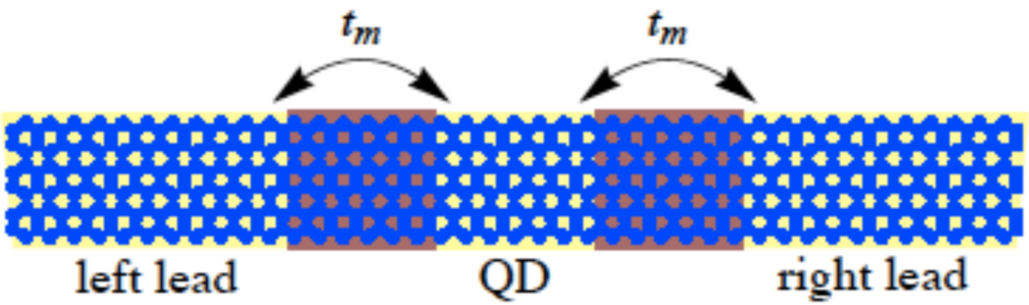
SU(N) Kondo: theoretical suggestions

SU(6) Coqublin-Schrieffer model in ultra-cold Yb



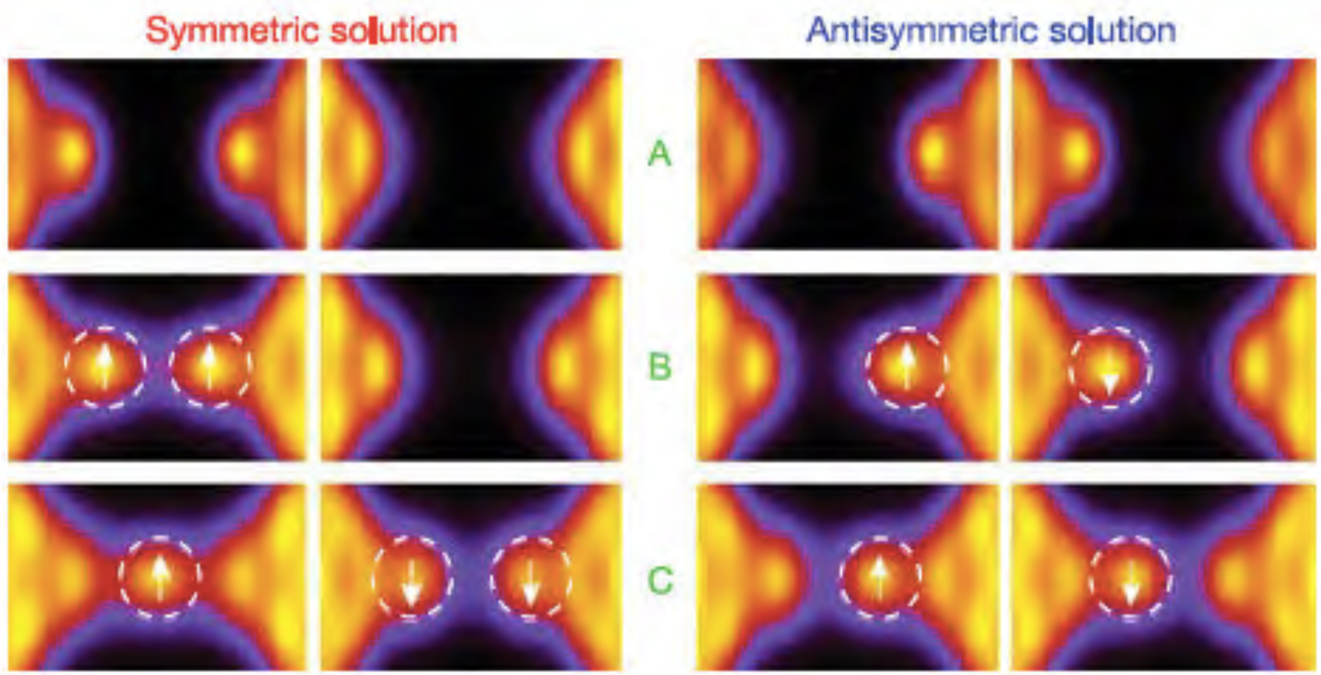
I. Kuzmenko, T. Kuzmenko, Y. Avishai, and G.-B Jo, PRB 2016

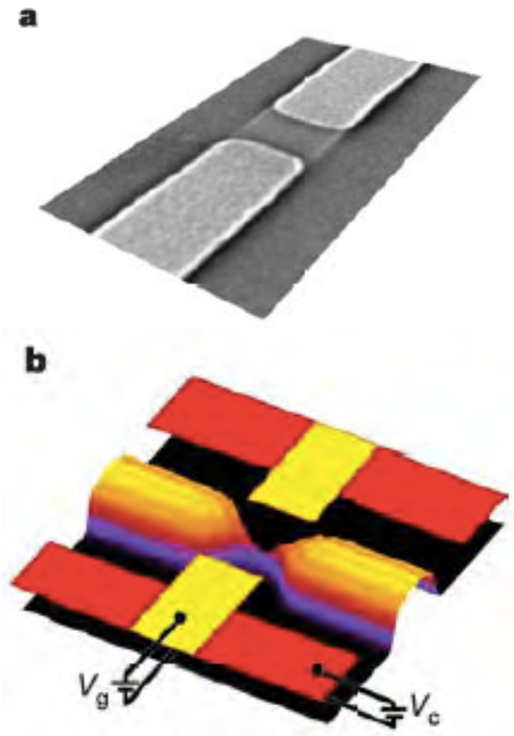
SU(12) Kondo effect in CNT -QD-CNT

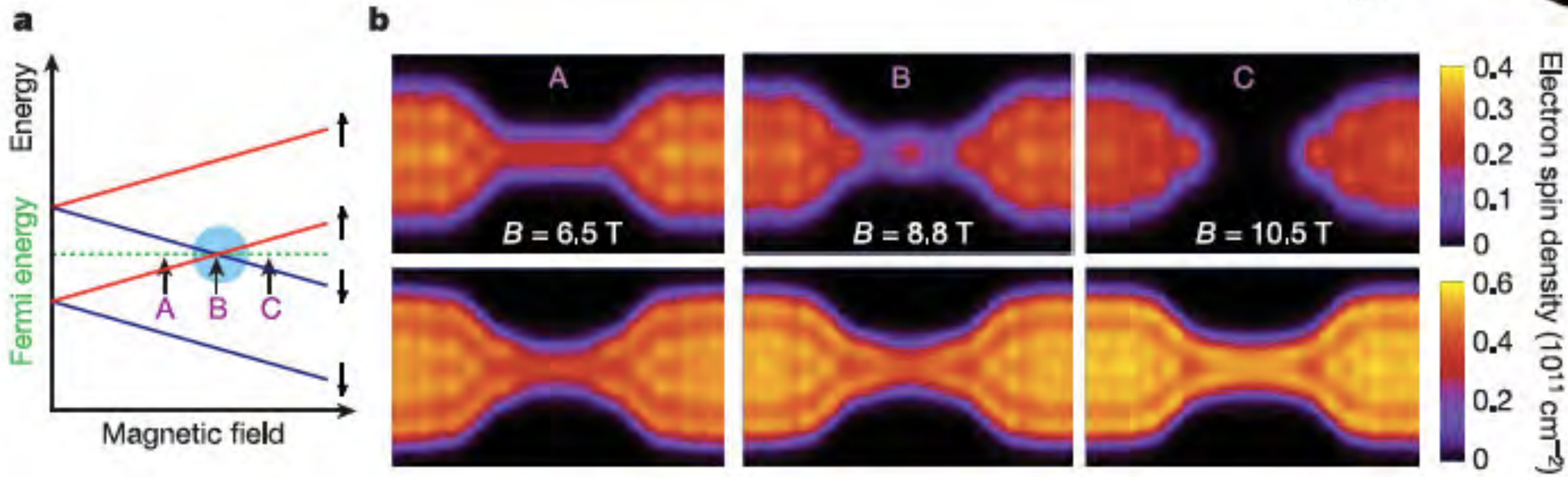


I. Kuzmenko and Y. Avishai PRB 2014

SU(2) ->SU(N) Kondo: 0.7 anomaly at QPC

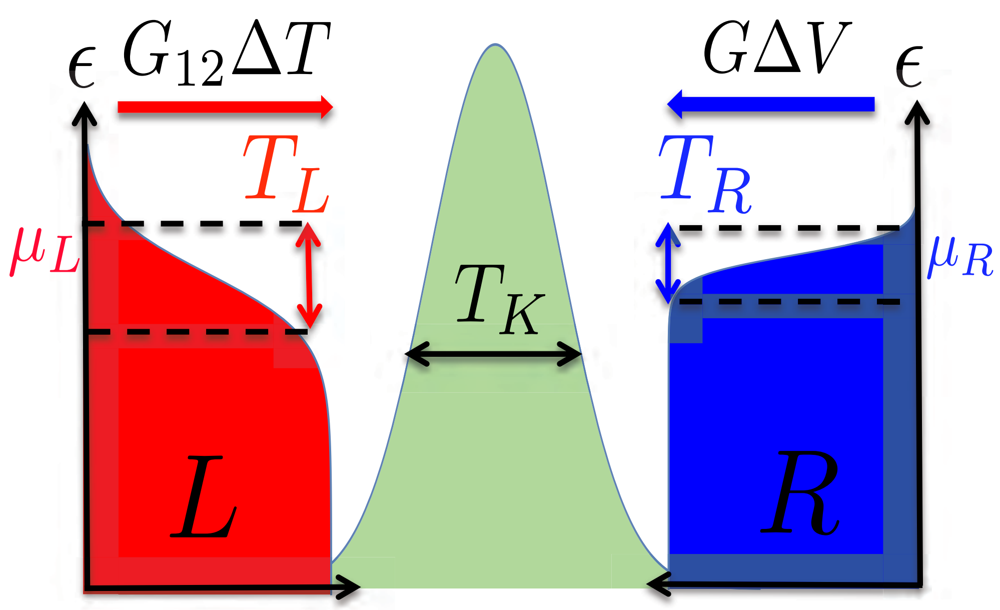


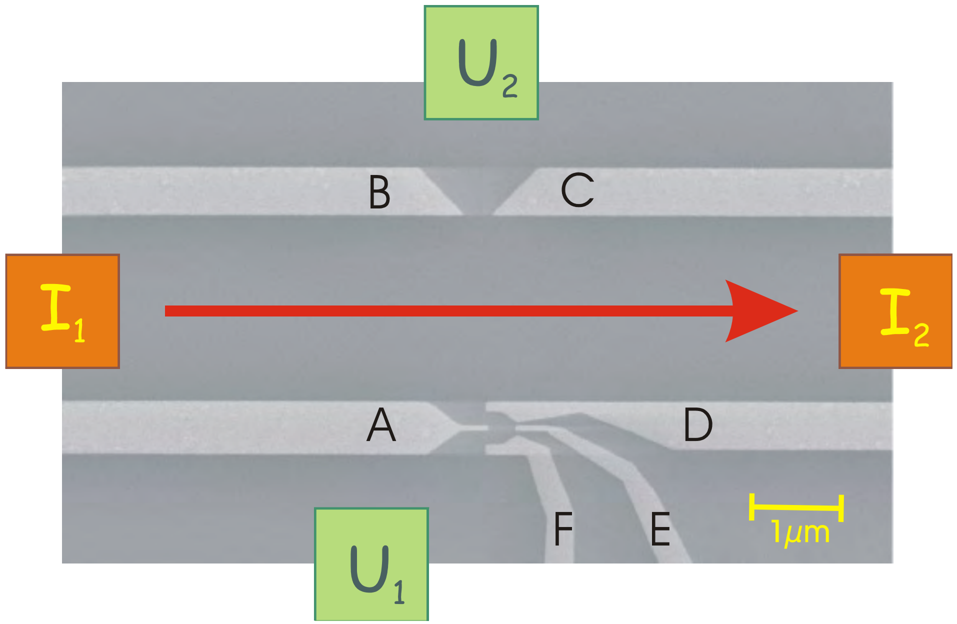




T. Rejec and Y. Meir, Nature 2006

How to develop a full fledged theory for Kondo-thermoelectrics at low temperatures ?





$$I = G \cdot V + G_{12} \cdot \Delta T = 0$$

Need to compute the thermopower the same way as it is measured in the experiment

Thermoelectrics of SU(N) Kondo: the model

$$H = \sum_{k\alpha r} \varepsilon_k c^\dagger_{\alpha k r} c_{\alpha k r} + \sum_r \epsilon_0 d^\dagger_r d_r + \sum_{r<r'} U d^\dagger_r d_r d^\dagger_{r'} d_{r'} + \sum_{k\alpha r} t_\alpha d^\dagger_r c_{\alpha k r} + h.c.$$

Schrieffer-Wolff transfromation

$$\boxed{\mathcal{H}_K = J_K^{\alpha\beta} \left(\mathbf{c}^\dagger_\alpha \lambda^\mu \mathbf{c}_\beta\right)\left(\mathbf{d}^\dagger \mathbf{\Lambda}^\mu \mathbf{d}\right)}$$

Glazman – Raikh rotation

$$a^\dagger = \frac{c^\dagger_L - c^\dagger_R}{\sqrt{2}}, \qquad b^\dagger = \frac{c^\dagger_L + c^\dagger_R}{\sqrt{2}}$$

Assume for simpicity
symmetric coupling
to the leads

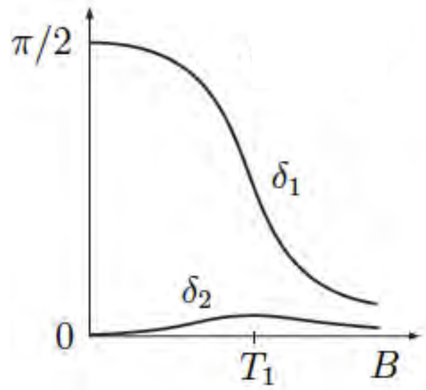
CFT

$$\mathcal{H}_K = -\lambda \ : \left(\mathbf{b}^\dagger \lambda^\mu \mathbf{b}\right) \cdot \left(\mathbf{b}^\dagger \lambda^\mu \mathbf{b}\right) :$$

$$\lambda \propto 1/T_K$$

P. Nozieres and A. Blandin, 1980
I. Affleck and A.W.W. Ludwig, 1991

Thermoelectrics of SU(N) Kondo: local FL



$$\delta(\varepsilon) = \delta_0 + \alpha_1 \varepsilon + ...$$

scattering (Friedel) phase

$$\alpha_1 = 1/T_K$$

$$H_0 = \nu \sum_r \int_\varepsilon \varepsilon \left[a^\dagger_{\varepsilon r} a_{\varepsilon r} + b^\dagger_{\varepsilon r} b_{\varepsilon r}\right]$$

Local Fermi Liquid

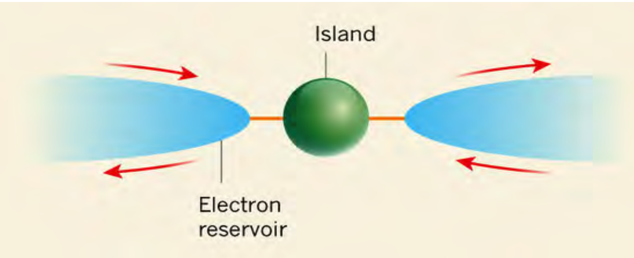
$$H_\alpha = -\sum_r \int_{\varepsilon_{1-2}} \left[\frac{\alpha_1}{2\pi}(\varepsilon_1 + \varepsilon_2) + \frac{\alpha_2}{4\pi}(\varepsilon_1 + \varepsilon_2)^2\right] b^\dagger_{\varepsilon_1 r} b_{\varepsilon_2 r}$$

$$H_\phi = \sum_{r<r'} \int_{\varepsilon_{1-4}} \left[\frac{\phi_1}{\pi\nu} + \frac{\phi_2}{4\pi\nu}\left(\sum_{i=1}^{4} \varepsilon_i\right)\right] : b^\dagger_{\varepsilon_1 r} b_{\varepsilon_2 r} b^\dagger_{\varepsilon_3 r'} b_{\varepsilon_4 r'} : .$$

$$\alpha_1 = (N-1)\phi_1$$
$$\alpha_2 = (N-1)\phi_2/4$$

Nozieres connections

Thermoelectrics of SU(N) Kondo: scattering basis



$$\hat{I}(x) = \frac{e\hbar}{2mi}\sum_{\sigma}\left[\psi_{\sigma}^{\dagger}(x)\partial_x\psi_{\sigma}(x) - \partial_x\psi_{\sigma}^{\dagger}(x)\psi_{\sigma}(x)\right]$$

$$\hat{I} = \frac{e}{2\nu h}\sum_{r}\left[a_r^{\dagger}(x)b_r(x) - a_r^{\dagger}(-x)Sb_r(-x) + H.c.\right],$$

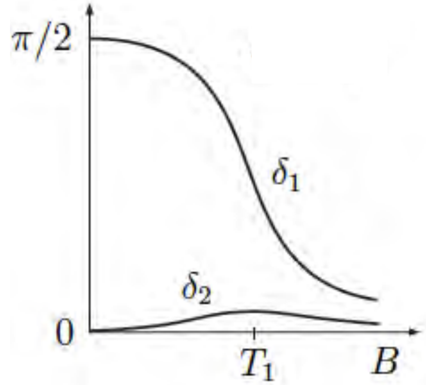
$$\psi_{a,k}(x) = \begin{cases} \sin\theta(e^{i(k_F+k)x} - e^{-i(k_F+k)x}) & x<0 \\ \cos\theta(e^{i(k_F+k)x} - e^{-i(k_F+k)x}) & x>0 \end{cases},$$

$$\theta = \pi/4 \qquad\qquad S_k = e^{2i\delta(\varepsilon_k)}$$

$$\psi_{b,k}(x) = \begin{cases} \cos\theta(e^{i(k_F+k)x} - S_k e^{-i(k_F+k)x}) & x<0 \\ \sin\theta(e^{-i(k_F+k)x} - S_k e^{i(k_F+k)x}) & x>0 \end{cases},$$

C. Mora et al, PRL, PRB 2007-2009

Thermoelectrics of SU(N) Kondo: Keldysh calculations



$$\alpha_1 = 1/T_K \qquad (T_L, T_R, eV) \ll T_K$$

Elastic current

$$I_{el} = \frac{Ne}{h}\int_{-\infty}^{\infty} d\varepsilon \mathcal{T}(\varepsilon)\Delta f(\varepsilon) \qquad \mathcal{T}(\varepsilon) = \sin^2\left[\delta(\varepsilon)\right] \qquad \delta(\varepsilon) = \delta_0 + \alpha_1\varepsilon + \ldots$$

$$\frac{I_{el}}{Ne/h} = \left[\sin^2\delta_0 + \frac{\alpha_1^2}{3}(\pi T)^2\cos 2\delta_0\right] e\Delta V - \left[\frac{\alpha_1}{3T}(\pi T)^2\sin 2\delta_0\right]\Delta T.$$

Inelastic current

$$\delta I_{in} = \langle T_C \hat{I}(t) e^{-i\int dt' H_\phi(t')}\rangle$$

$$\delta I_{in} = \mathcal{S}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\left(\Sigma^{-+}(\varepsilon) - \Sigma^{+-}(\varepsilon)\right) i\pi\nu\Delta f(\varepsilon)$$

Thermoelectrics of SU(N) Kondo: conductance and thermoelectric coefficient

Linear response

$$G(T) = G_0\left[\sin^2\delta_0 + \frac{\alpha_1^2}{3}\frac{N+1}{N-1}(\pi T)^2\cos 2\delta_0\right]$$

$$G_{12}(T) = -G_0\left[\frac{\alpha_1}{3e}\pi^2 T\sin 2\delta_0\right],$$

thermopower $\boxed{S = -\frac{V}{\Delta T}} = \frac{G_{12}}{G}$

$$S(T) = -2eL_0 T\cot\tilde{\delta}_0 \left.\frac{\partial\tilde{\delta}(\varepsilon)}{\partial\varepsilon}\right|_{\varepsilon=0} = -\frac{\pi T}{eT_K(N)}\cot\tilde{\delta}_0,$$

$$SU(N)\big|_{N=4} \quad \delta_0^m = \frac{\pi m}{N}$$

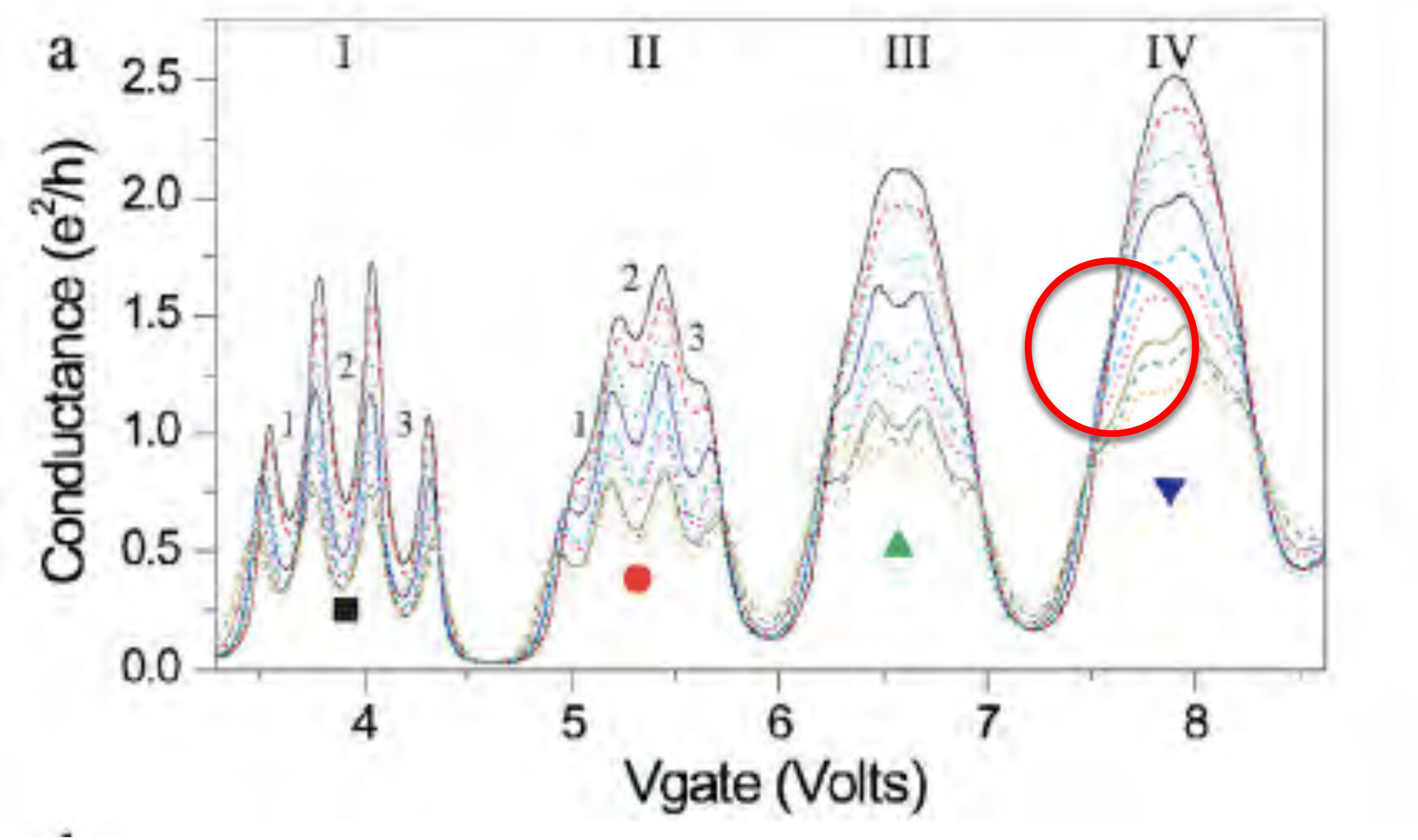
$m = 1 \quad \delta_0 = \pi/4$

$m = 2 \quad \delta_0 = \pi/2$

Thermoelectrics of SU(4) Kondo: important check

$$G(T) = G_0 \left[\sin^2 \delta_0 + \frac{\alpha_1^2}{3} \frac{N+1}{N-1} (\pi T)^2 \cos 2\delta_0 \right]$$

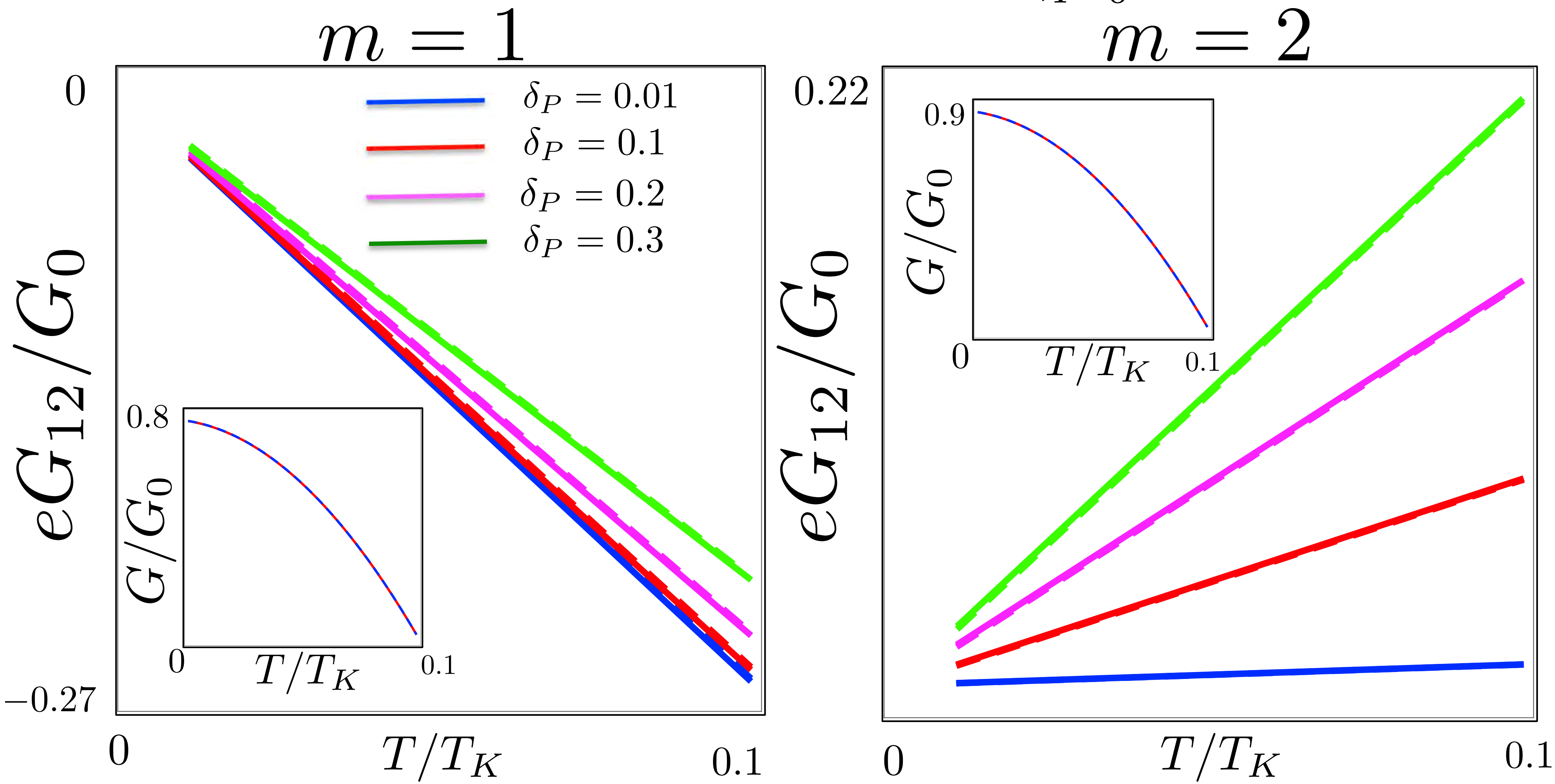
$$G_{12}(T) = -G_0 \left[\frac{\alpha_1}{3e} \pi^2 T \sin 2\delta_0 \right],$$



Thermoelectrics of SU(N) Kondo: results

Linear response

Differential TP: $S(T) = -\lim_{\Delta T \to 0} \frac{V}{\Delta T}\Big|_{I=0} = \frac{G_{12}(T)}{G(T)}$



$$I = G \cdot V + G_{12} \cdot \Delta T = 0$$

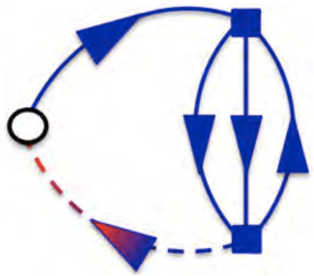
Thermoelectrics of SU(N) Kondo: results

Beyond the linear response $(T_L, T_R, eV) \ll T_K$

Elastic current $$I_{el} = \frac{Ne}{h}\int_{-\infty}^{\infty} d\varepsilon \mathcal{T}(\varepsilon)\Delta f(\varepsilon)$$

$$\mathcal{T}(\varepsilon) = \sin^2\left[\delta(\varepsilon)\right] \qquad \delta_r(\varepsilon) = \delta_0 + \alpha_1\varepsilon + \alpha_2\left(\varepsilon^2 - \mathcal{A}\right)$$

$$\mathcal{A} = \left[\frac{(e\Delta V)^2}{4} + \frac{(\pi T)^2}{3} + \frac{\pi^2 T\Delta T}{3}\right]$$



Inelastic current $$\delta I_{in} = \mathcal{S}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\left(\Sigma^{-+}(\varepsilon) - \Sigma^{+-}(\varepsilon)\right) i\pi\nu\Delta f(\varepsilon)$$

$$\Sigma^{\eta_1,\eta_2}(t) = \left(\frac{\phi_1}{\pi\nu^2}\right)^2 \sum_{k_1,k_2,k_3} G_{bb}^{\eta_1,\eta_2}(k_1,t)G_{bb}^{\eta_2,\eta_1}(k_2,-t)G_{bb}^{\eta_1,\eta_2}(k_3,t)$$

$$G_{bb}^{+-}(t) = -\frac{\pi\nu}{2}\left[\frac{T_L e^{-i\mu_L t}}{\sinh(\pi T_L t)} + \frac{T_R e^{-i\mu_R t}}{\sinh(\pi T_R t)}\right]$$

$$\delta I_{in} = \frac{N(N-1)e\pi}{2h}\left(\frac{\phi_1}{\pi\nu^2}\right)^2 2\cos 2\delta_0\left(\frac{\pi\nu}{2}\right)^4 \times \{[\mathcal{L}(T_L,T_R,z) - \mathcal{L}(T_L,T_R,0)] - [\mathcal{L}(T_R,T_L,-z) - \mathcal{L}(T_R,T_L,0)]$$

$$\mathcal{L}(x,y,z) = \int_{-\infty-i\gamma}^{+\infty-i\gamma}\left[\frac{x^4}{\sinh^4(\pi x t)} + 2x^3 y\frac{e^{izt}}{\sinh^3(\pi x t)\sinh(\pi y t)} + x^2y^2\frac{e^{2izt}}{\sinh^2(\pi x t)\sinh^2(\pi y t)}\right]dt$$

Summing up (so far):

- We developed a theoretical method for calculation of the charge

  current $I(T_L, T_R, V)$ using the non-equilibrium Keldysh approach

- Assuming the zero current steady state condition

  $I(T_L, T_R, V) = 0$ we solve a non-linear equation for $V(T_L, T_R)$

- We find the thermoelectric power (Seebeck effect) $S = \frac{V(T_L, T_R)}{T_L - T_R}$

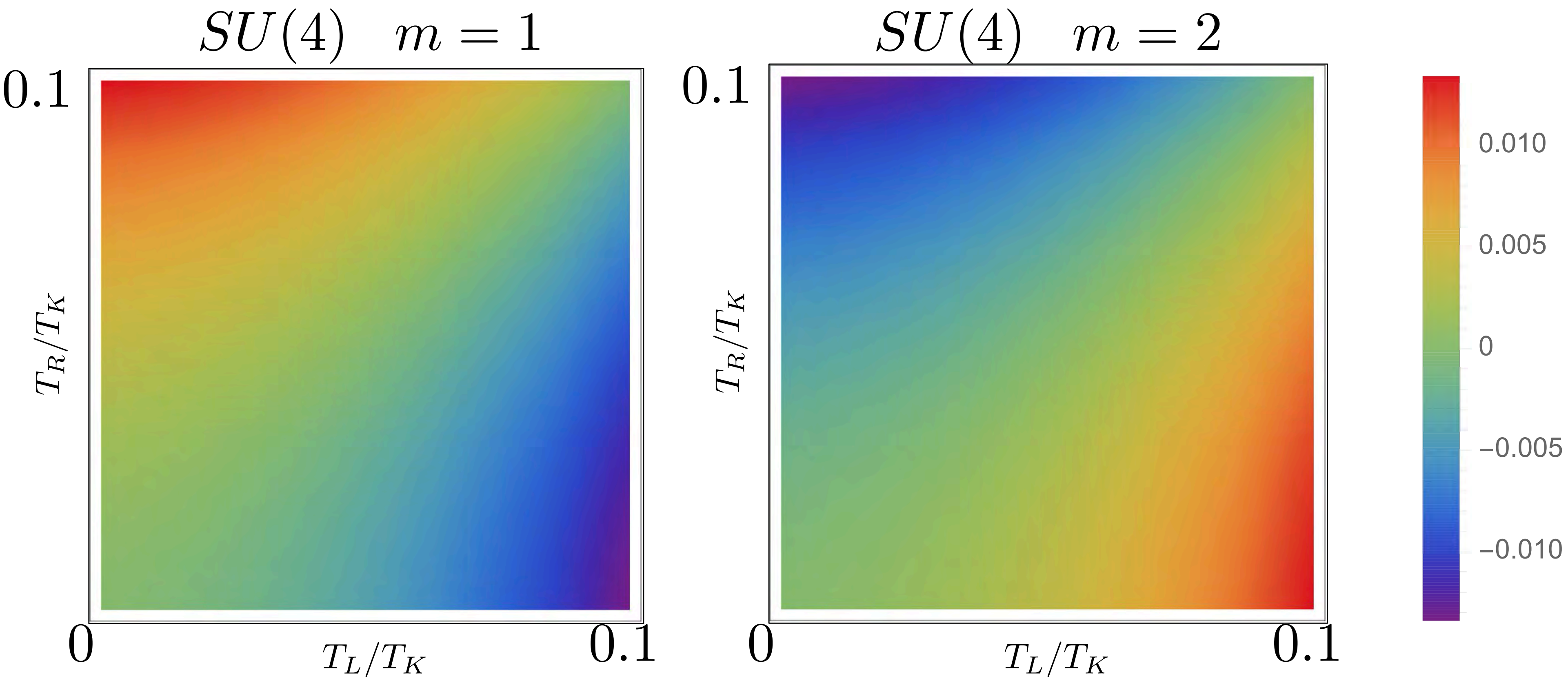
which is valid beyond the linear response theory

- We compare it with the linear response differential thermopower

$$S = \lim_{T_L \to T_R} \frac{V(T_L, T_R)}{T_L - T_R}$$

- The method exactly follows the experimental way of measuring TP

Thermoelectrics of SU(N) Kondo: results



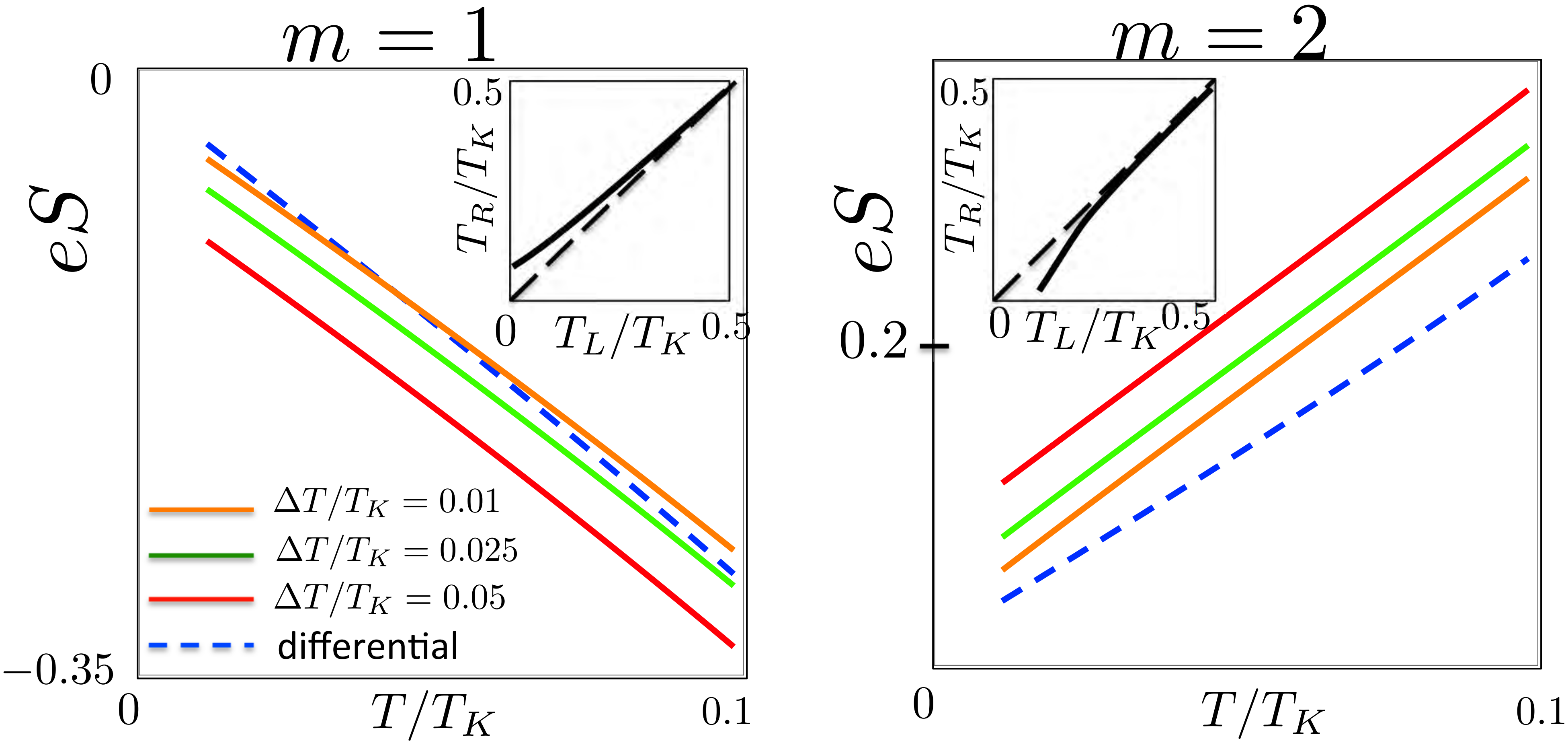
thermopower

$$\boxed{S = -\frac{V}{\Delta T}} = \frac{G_{12}}{G}$$

$$I = G \cdot V + G_{12} \cdot \Delta T = 0$$

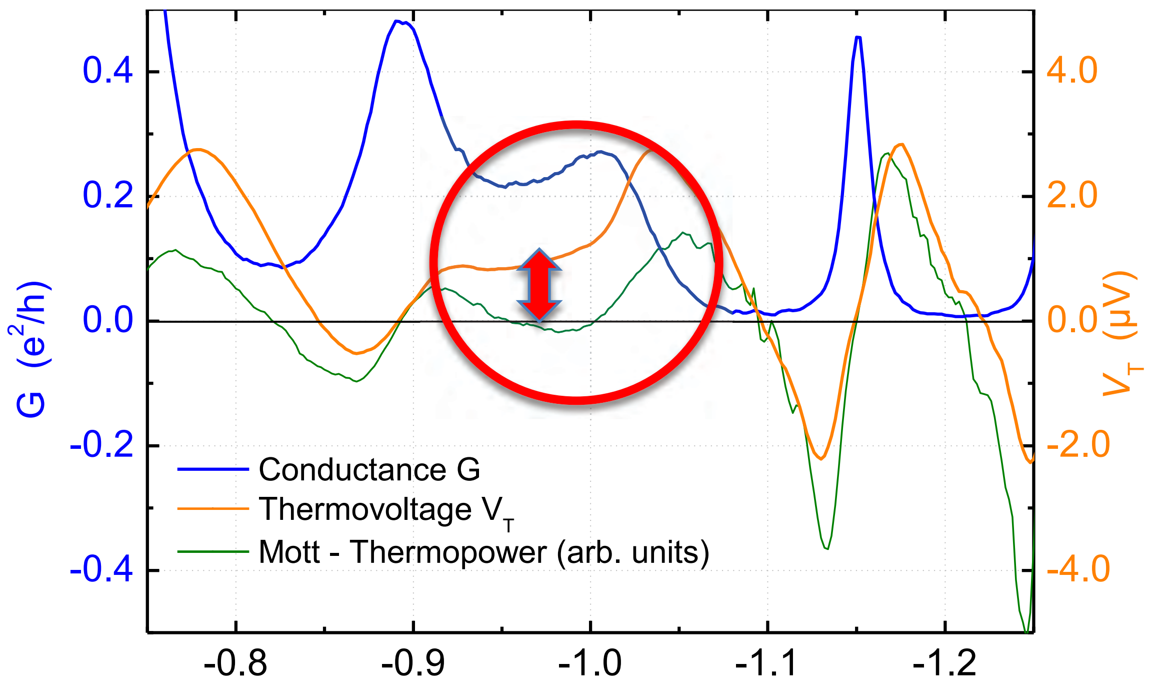
Thermoelectrics of SU(N) Kondo: results

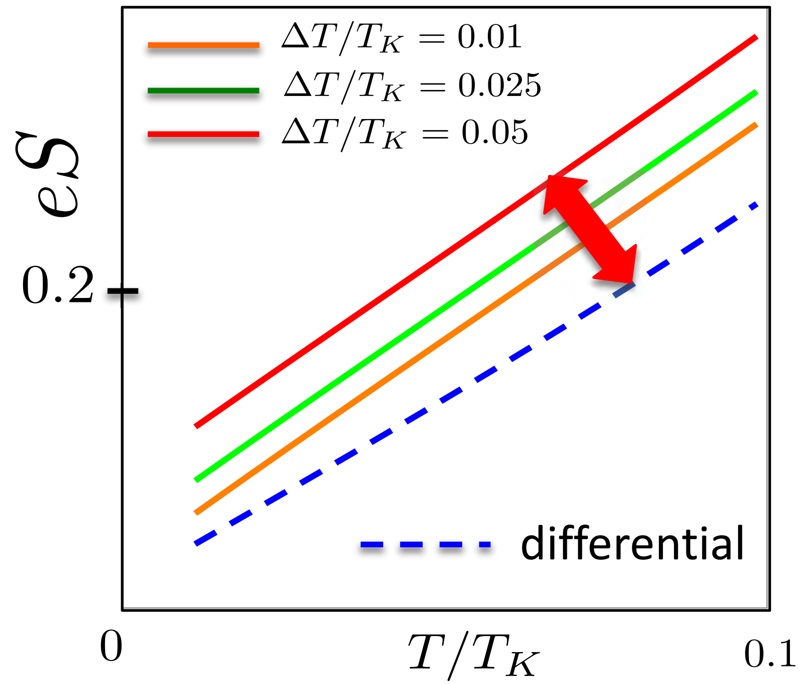
$$S = -\frac{V}{\Delta T}$$



$$I = G \cdot V + G_{12} \cdot \Delta T = 0$$

Thermoelectrics of SU(N) Kondo: explanation for the puzzle ?





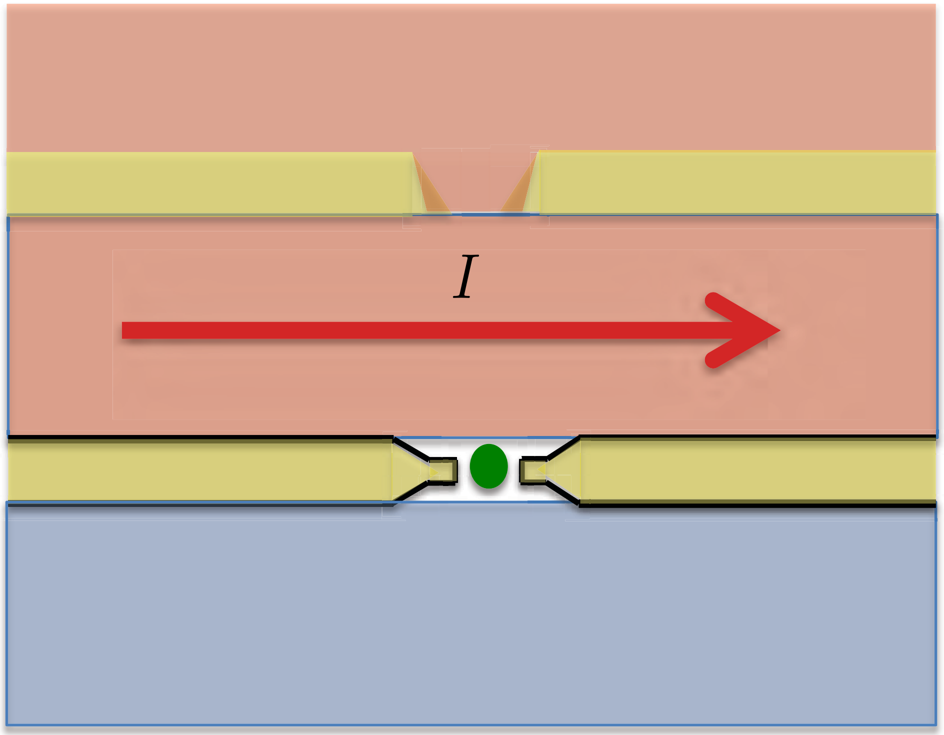
$$I = G \cdot V + G_{12} \cdot \Delta T = 0$$

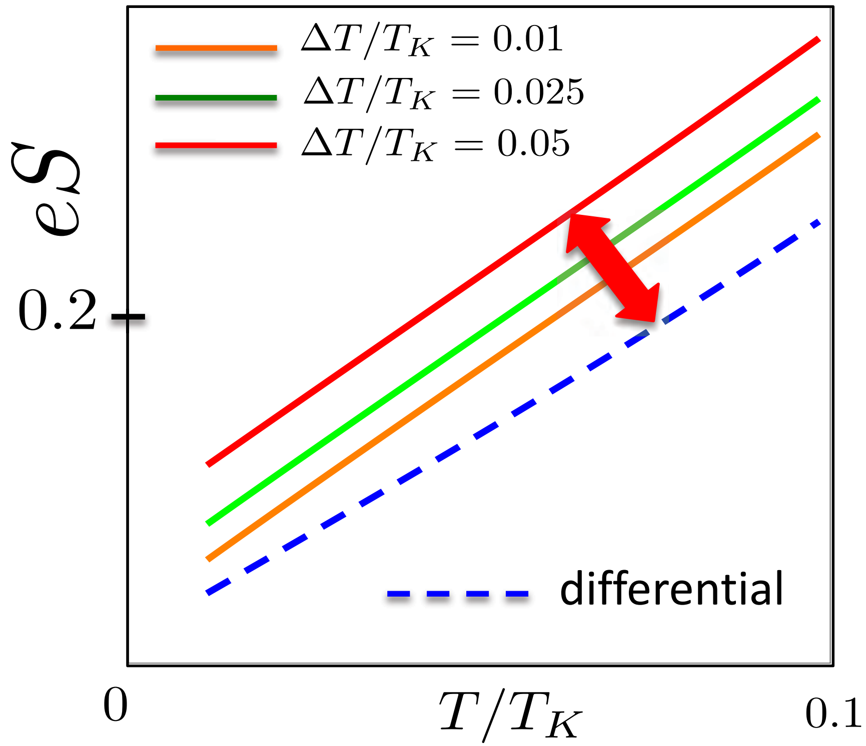
additional experiments needed

From the “Heaven” to the “Earth”:

designing the new experiments

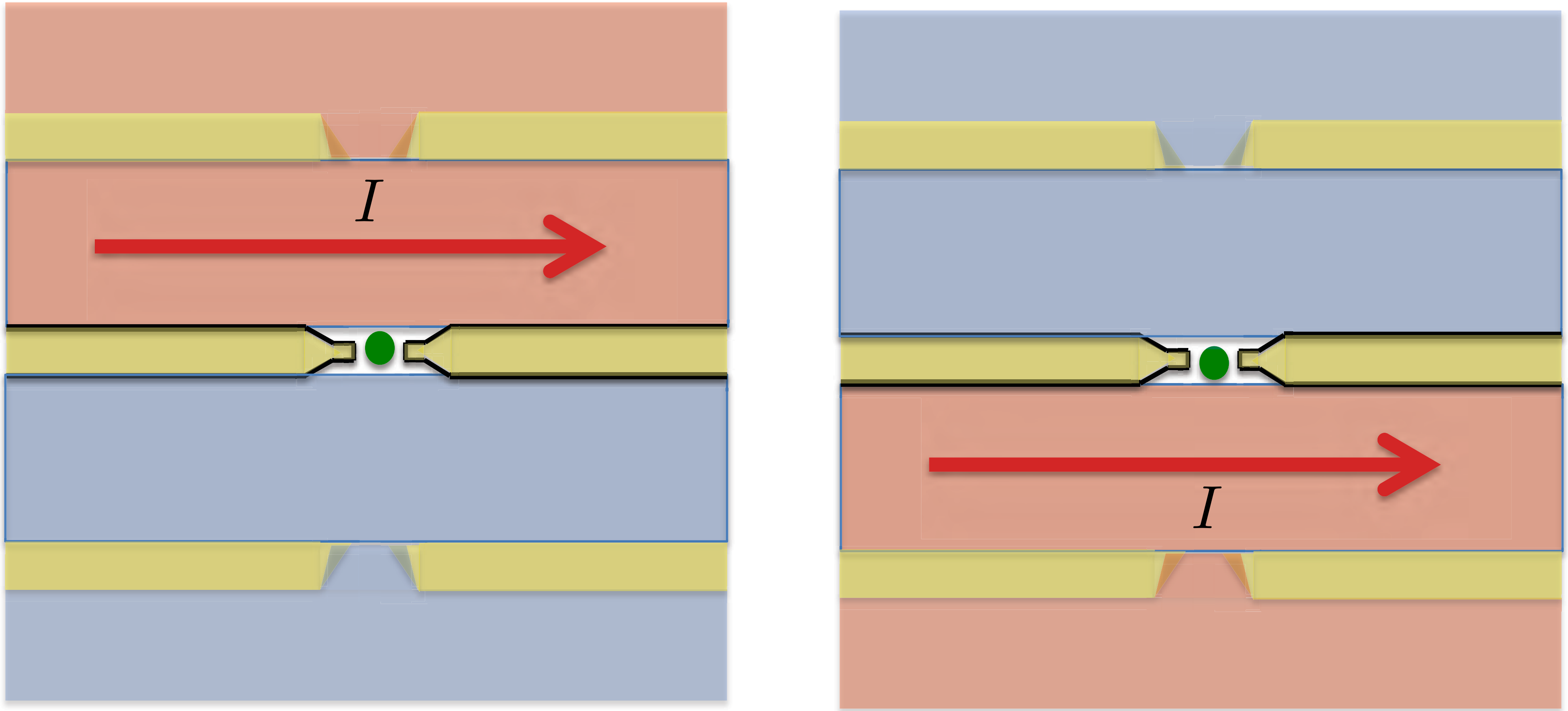
Suggestions: how to check the offset?





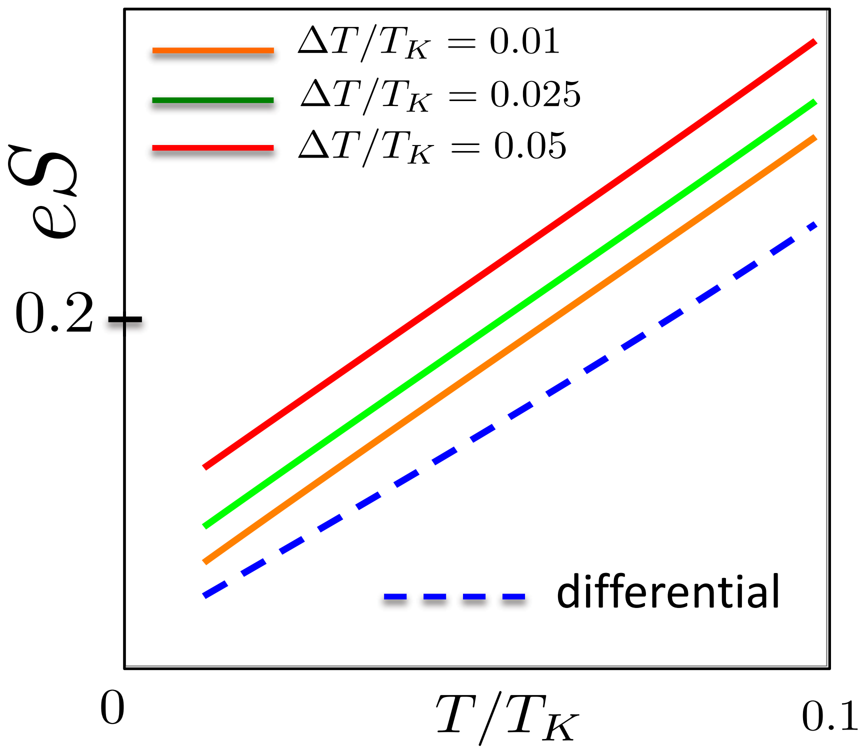
Message 1: Perform experiments at different currents (different temperature drops between the leads)

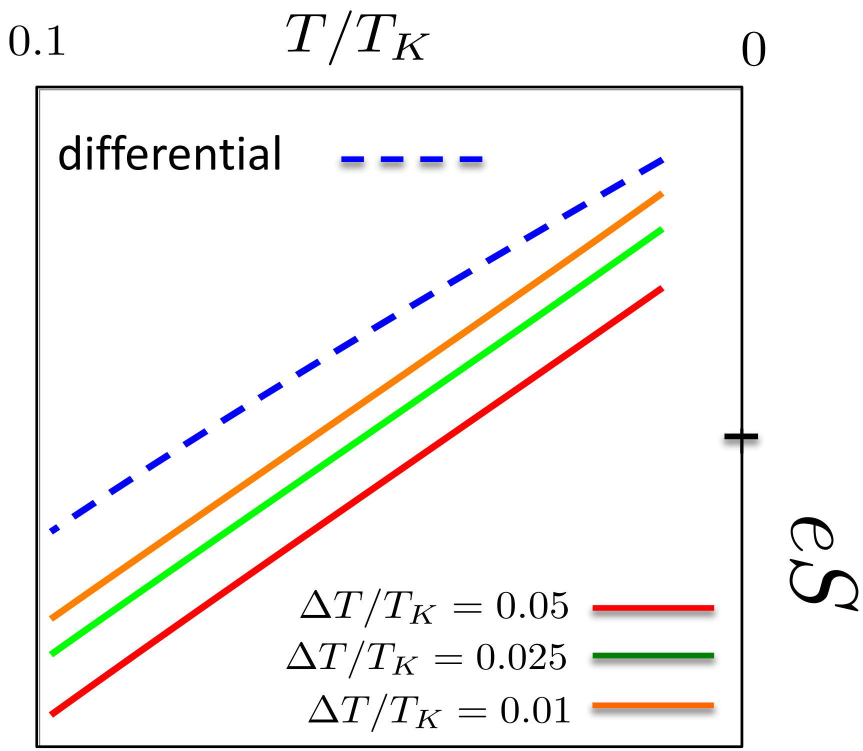
Suggestions: how to check the offset?



Message 2: Perform experiments inverting the sign of the temperature drop

Suggestions: how to check the offset?

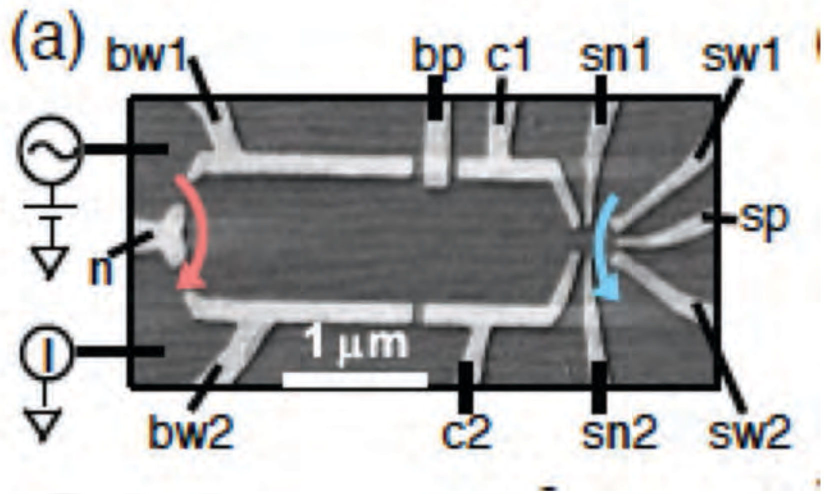




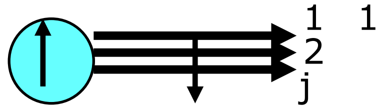
Message 3: Results should depend on the sign of ΔT !

Use it for measuring the temperature of hot contact !

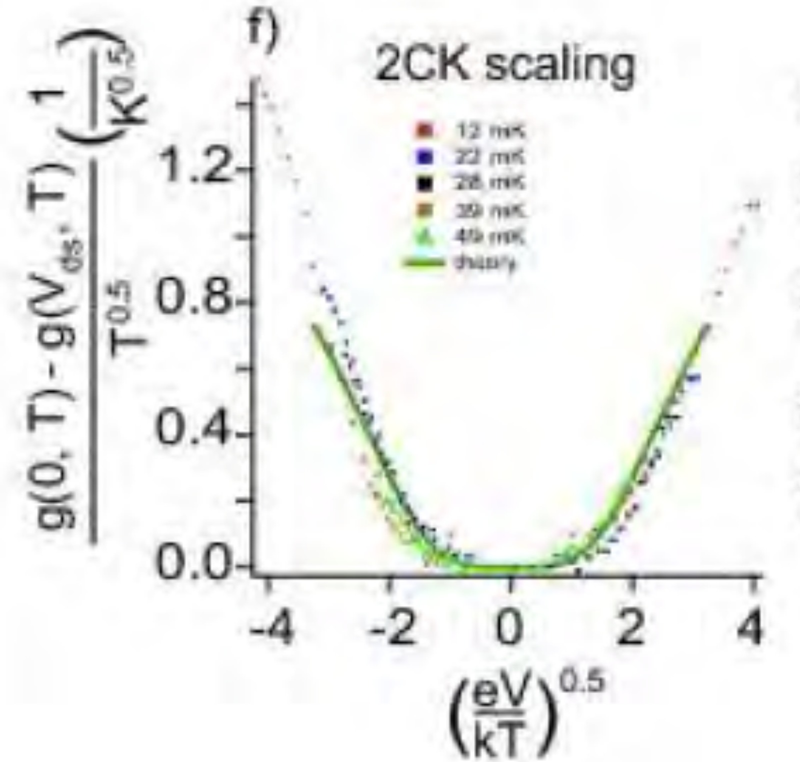
What about local SU(N) non-Fermi liquids?

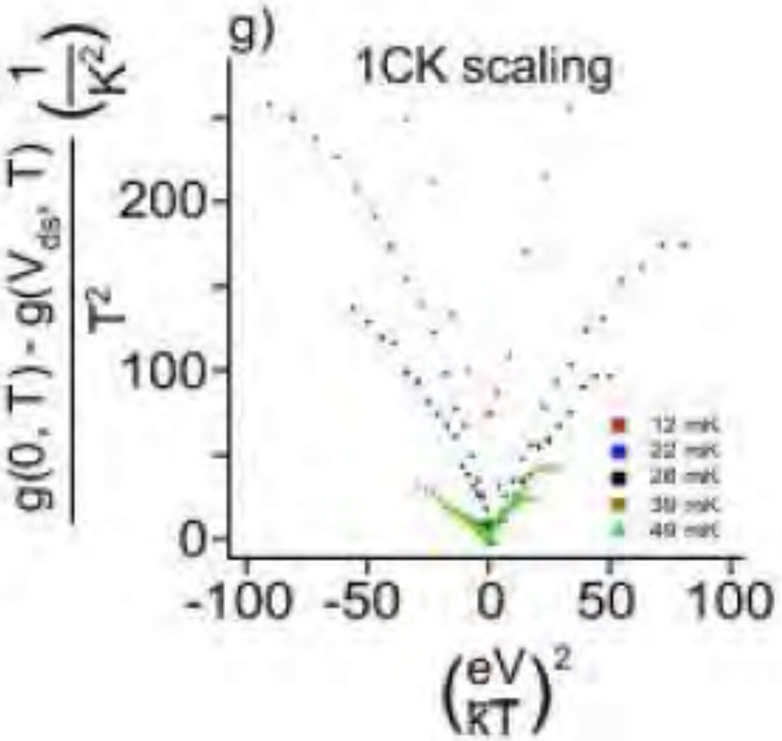


$$J\sum_j c^+_{j\sigma}\vec{\sigma}_{\sigma\sigma'}c_{j\sigma'}\vec{S}$$



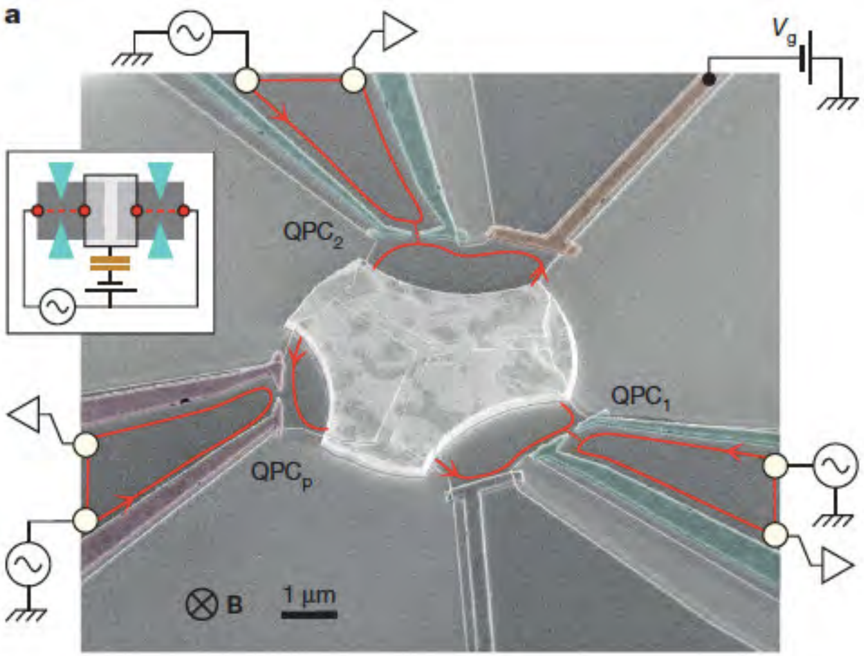
$$g(V_{\rm ds}) \sim {\rm const} - \sqrt{eV_{\rm ds}}$$



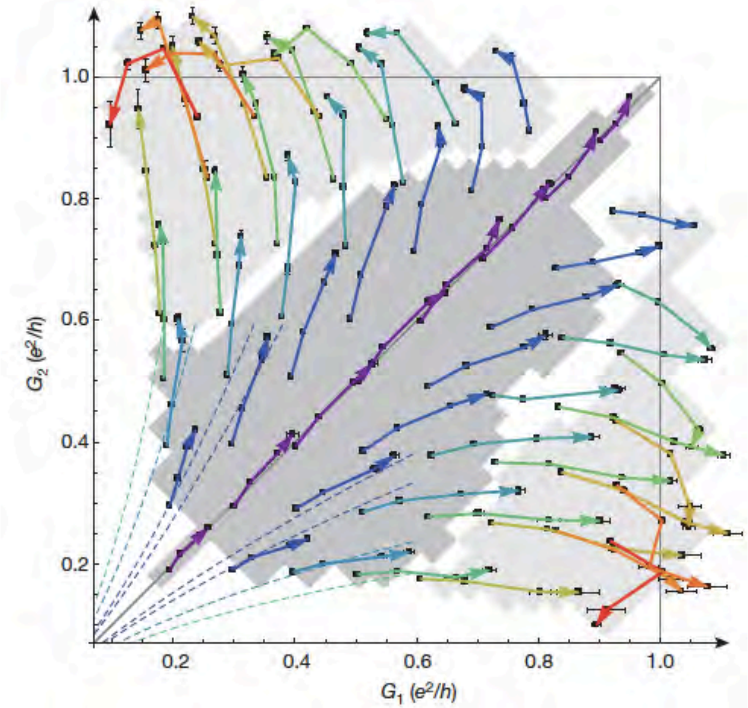


R.M. Potok et al, Nature, 2007

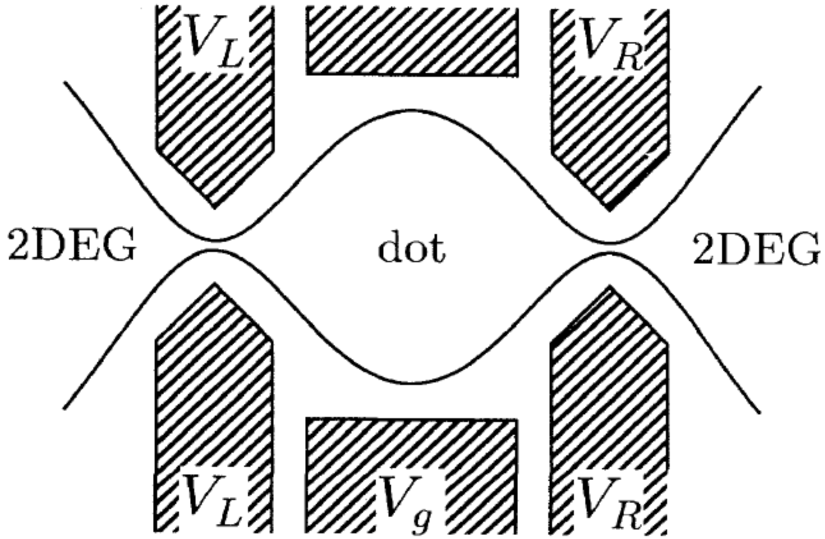
Two-channel charge Kondo effect



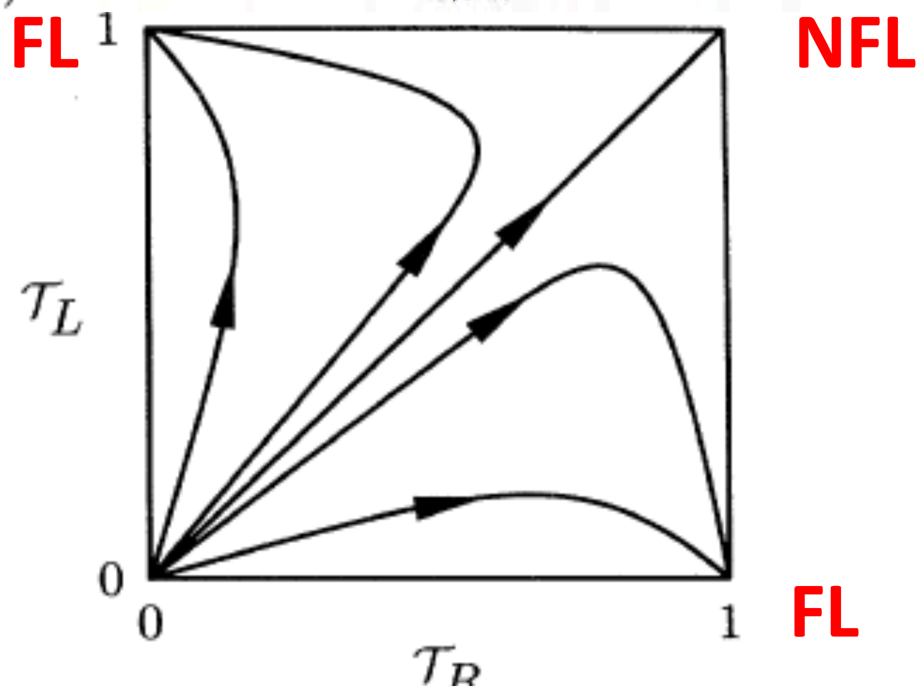
Z. Iftikhan et al, Nature 526 (2015)



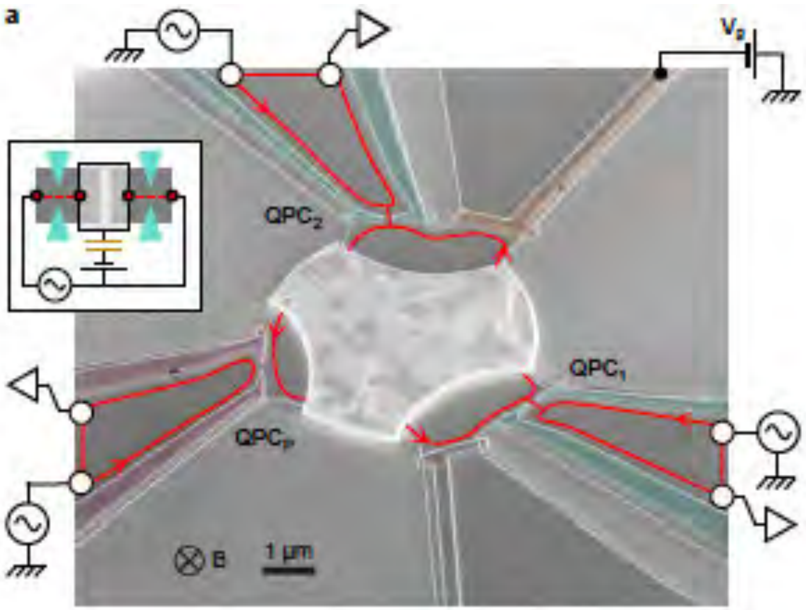
(a)

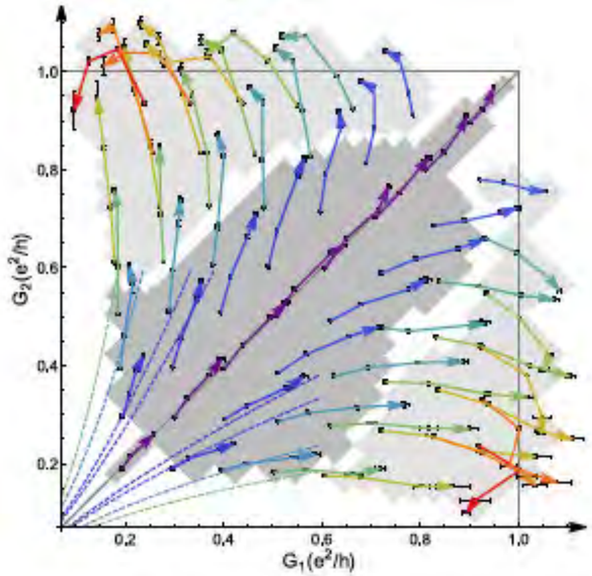


A.Furusaki and K.A.Matveev, PRB 52 (1995)

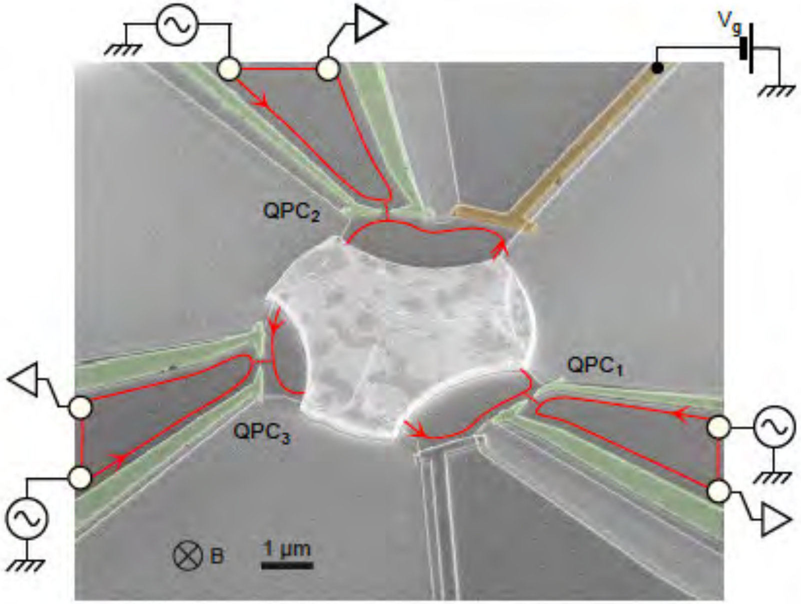


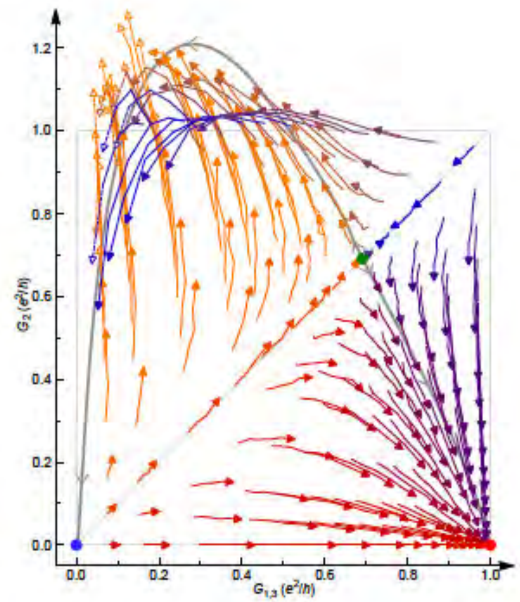
Parafermion states with multi-channel Kondo effect





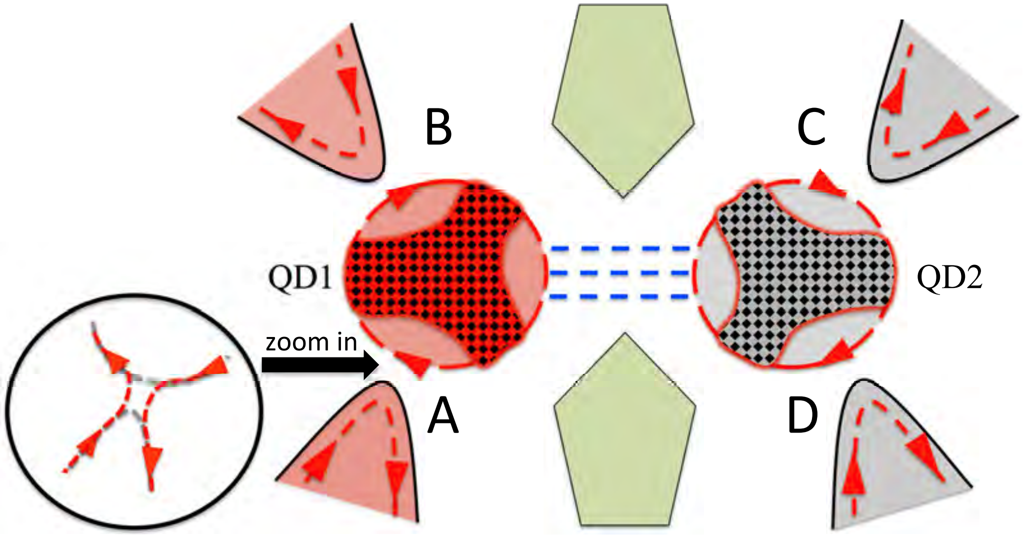
Z_2



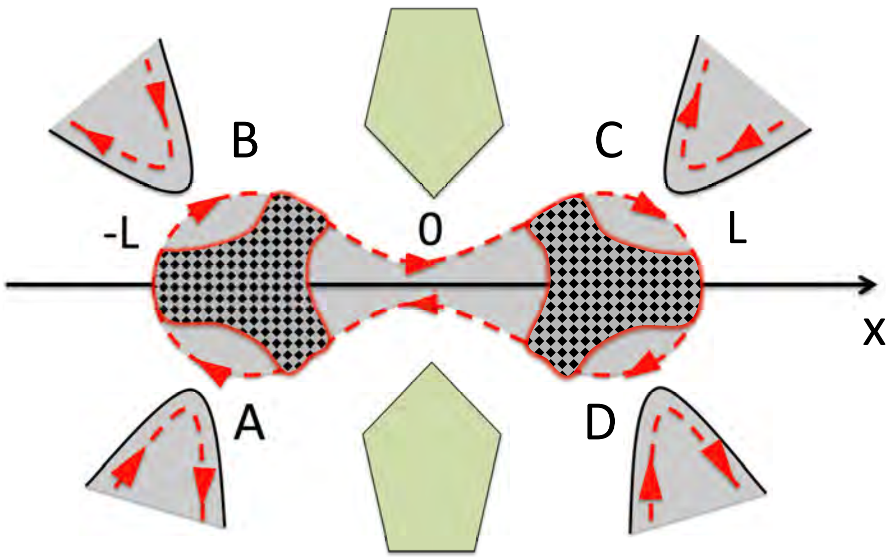


Z_3

Weak link between Fermi and non-Fermi liquids

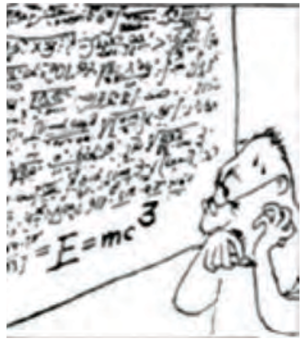


Two-Impurity non-Fermi liquid driven by Kondo



T. K. T. Nguyen and MK, PRB 97, 085403 (2018)

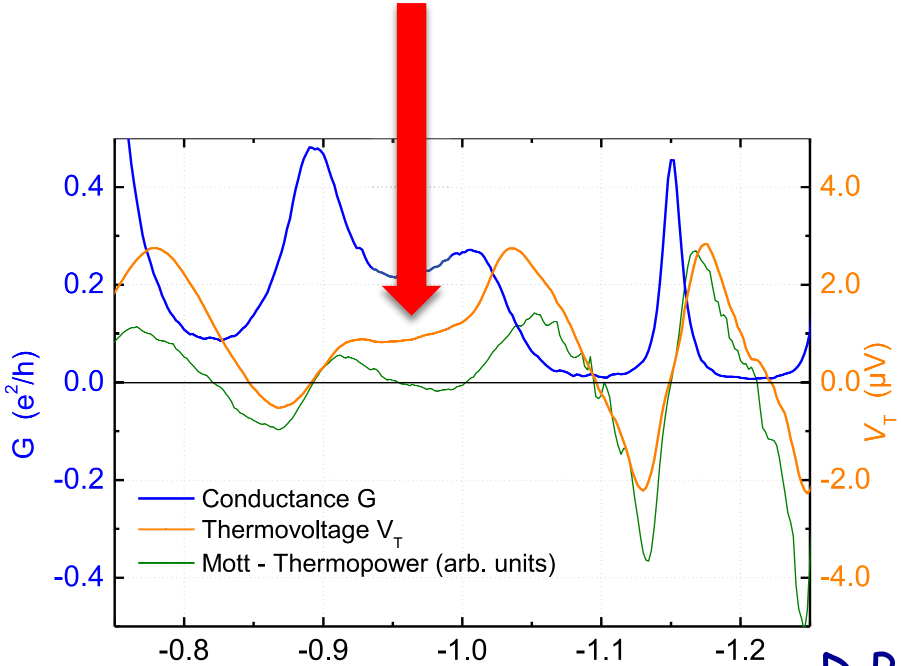
Take home messages

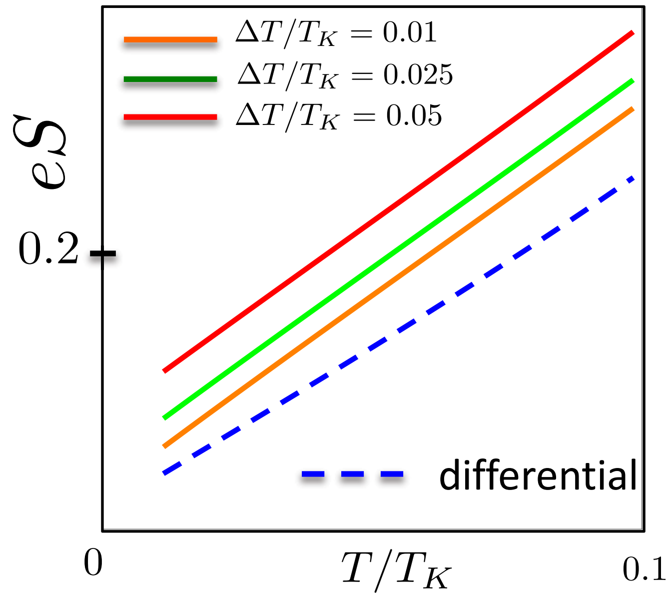


- Thermopower is maximal in the particle-hole non-symmetric SU(N) regime with minimal (electrons) or maximal (holes) filling factors

$$\mathrm{e}\, S(T) \propto \frac{N \cdot T}{T_K(N)} \quad \text{at} \quad N \gg 1$$

- Non-linear in temperature drop effects are significant at low temperatures and lead to enhancement of the Seebeck effect





D.B. Karki and MK PRB B **96**, 121403(R) 2017

Thank you!

The Abdus Salam
International Centre
for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency