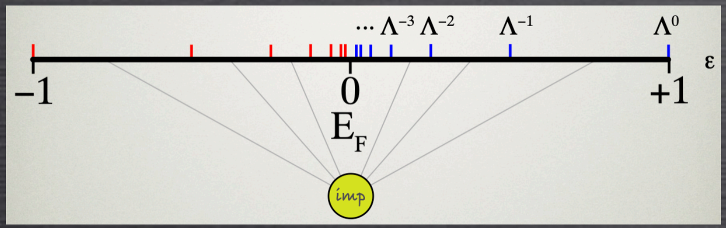
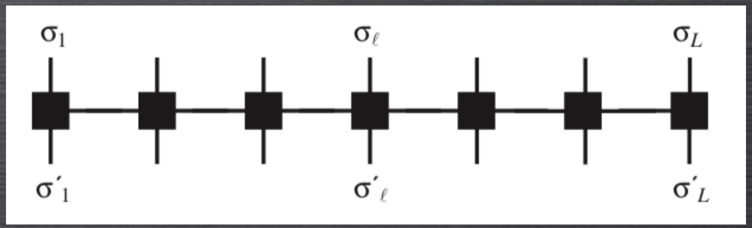
Solvers for quantum impurity problems (with superconducting baths)

Lecture 1: General introduction





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Contents and goals

- quantum impurity physics
- many-body effects (Kondo)
- numerical renormalization group (NRG)
- tensor networks & DMRG
- superconducting systems and sub-gap states

- "NRG Ljubljana" implementation
- DMRG for Richardson's equation

- other impurity solvers (e.g. quantum Monte Carlo)
- computer algebra in Mathematica (SNEG)
- linear algebra, C++, HPC, parallelization issues,...

Literature

Hewson: The Kondo problem to heavy fermions, Cambridge University Press (1993)
Wilson: The renormalization group: Critical phenomena and the Kondo problem, Rev. Mod. Phys. 47, 773 (1975)
Krishnamurthy, Wilkins, Wilson: Renormalization-group approach to the Anderson model of dilute magnetic alloys. I. Static properties for the symmetric case, Phys. Rev. B 21, 1003 (1980)
Krishnamurthy, Wilkins, Wilson: Renormalization-group approach to the Anderson model of dilute magnetic alloys. II. Static properties for the asymmetric case, Phys. Rev. B 21, 1044 (1980)
Satori, Shiba, Sakai, Shimizu: Numerical Renormalization Group Study of Magnetic Impurities in Superconductors, J. Phys. Soc. Japan, 61, 3239 (1992)
Bulla, Costi, Pruschke: Numerical renormalization group for quantum impurity systems, Rev. Mod. Phys. 80, 395 (2008)
Schöllwock: The density-matrix renormalization group in the age of matrix product states, Annals of Physics, 326, 96 (2011)
ITensor tutorials, http://itensor.org/docs.cgi?page=tutorials&vers=cppv3
Pavesic, Bauernfeind, Zitko: Yu-Shiba-Rusinov states in superconducting islands with finite charging energy, arxiv:2101.10168
Gull et al., Continuous-time Monte Carlo methods for quantum impurity models, Rev. Mod. Phys. 83, 349 (2011)

Precompiled codes

Singularity containers (OS-level virtualization)

http://f1web.ijs.si/~zitko/containers/singularity_for_CPH/

foss-2020a.sif container (CentOS 7.7 + all libraries)
nrgljubljana/ two versions of NRG code
tensor/ DMRG code for Richardson model
ctqmc/ CT-HYB QMC code

Materials

Presentations + examples

http://f1web.ijs.si/~zitko/courses/2021_CPH/

Quantum impurity

- point-like object with a local degree of freedom
  example: spin & orbital angular momentum of a magnetic dopant atom
- environment = continuum of states
  example: itinerant electrons in a metal
- interaction that can change the value of local d.o.f.
  example: exchange coupling & spin-flip scattering

SPIN-BOSON MODEL

$|0\rangle$ $\qquad$ $|1\rangle$

two-level system, "spin"

continuum (sea) of levels

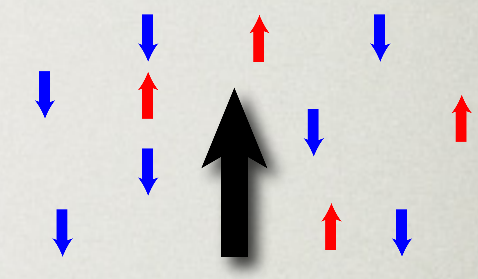
$$H = \Delta\sigma_x + \sum_i \left(\frac{p_i^2}{2m} + \frac{1}{2} m\omega_i^2 x_i^2 \right) + \sigma_z \sum_i c_i x_i$$

model for studying decoherence and quantum dissipation

U. Weiss: Quantum dissipative systems (3rd ed, 2008)

Kondo model

$$H = H_{\rm band} + H_{\rm exch}$$



$$H_{\rm band} = \sum_{\mathbf{k},\sigma} \epsilon_k \, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

Fermi sea: gas of
non-interacting electrons

$$H_{\rm exch} = J \, \mathbf{S} \cdot \mathbf{s}$$

exchange
coupling

$$\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$$ quantum-mechanical spin operator

$$\mathbf{s} = \frac{1}{N}\sum_{kk'} c^\dagger_k \left(\frac{1}{2}\boldsymbol{\sigma}\right) c_{k'} = f^\dagger_0 \left(\frac{1}{2}\boldsymbol{\sigma}\right) f_0$$ spin-density (at **r**=0)

(Zener, 1951)

Single-Impurity Anderson model

$$H = H_{\text{imp}} + H_{\text{band}} + H_{\text{hyb}}$$

$$H_{\text{imp}} = \sum_{\sigma} \epsilon\, n_{\sigma} + U\, n_{\uparrow} n_{\downarrow} \qquad n_{\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$$

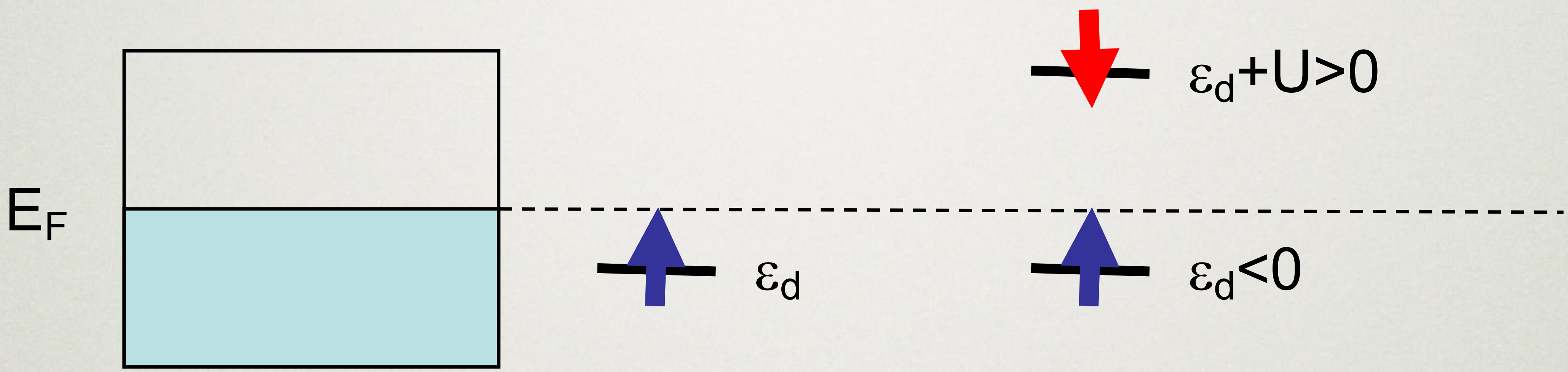
$$H_{\text{band}} = \sum_{\mathbf{k},\sigma} \epsilon_k\, c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma}$$

$$H_{\text{hyb}} = \sum_{k,\sigma} \Big(V_k\, c_{k,\sigma}^{\dagger} d_{\sigma} + \text{H.c.} \Big)$$

$$\Delta(z) = \sum_k \frac{|V_k|^2}{z - \epsilon_k} \approx -i\Gamma \qquad z = \omega + i\delta,\ \delta > 0,\ \delta \to 0$$

$$\pi \sum_k |V_k|^2 \delta(\omega - \epsilon_k) \approx \pi |V|^2 \sum_k \delta(\omega - \epsilon_k) = \pi |V|^2 \rho = \Gamma$$

Emergence of local moment in SIAM

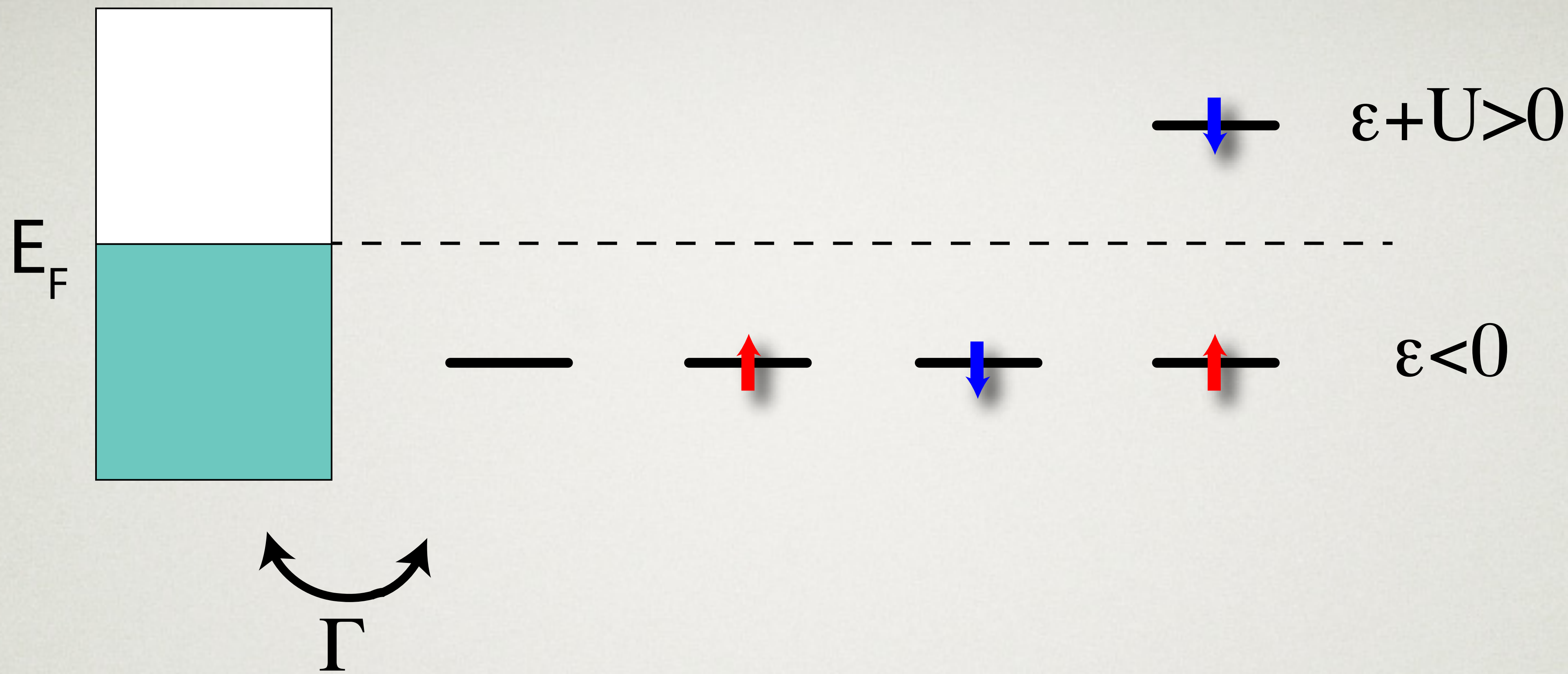


Localized Magnetic States in Metals

P. W. Anderson
Phys. Rev. **124**, 41 – Published 1 October 1961

Article | References | Citing Articles (3,556) | PDF | Export Citation

Nobel prize in 1977 (with Mott and Van Vleck): "for their fundamental theoretical investigations of the electronic structure of **magnetic** and disordered systems."



$$\boxed{\delta} = \epsilon + U/2$$

δ=0 is a special “particle-hole symmetric point” with ⟨n⟩=1

$$\rho J = \frac{8U}{\pi\Gamma}$$ Schrieffer-Wolff transformation

Schrieffer, Wolff, Phys. Rev. (1966)
Bravyi, DiVincenzo, Loss, Ann. Phys. (2011)

(Quantum-mechanical) spin

$$[S^i, S^j] = i\epsilon_{ijk} S^k$$

$$\mathbf{S}^2 |s, m\rangle = s(s+1)|s, m\rangle$$

$$S^z |s, m\rangle = m|s, m\rangle$$

$$S^+ |s, m\rangle = \sqrt{s(s+1) - m(m+1)}|s, m+1\rangle$$

$$S^- |s, m\rangle = \sqrt{s(s+1) - m(m-1)}|s, m-1\rangle$$

$$S^+ = S^x + iS^y$$

$$S^- = S^x - iS^y$$

Spin-1/2

$$\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\mathbf{S} = \frac{1}{2}\begin{pmatrix} d_\uparrow^\dagger & d_\downarrow^\dagger \end{pmatrix} \boldsymbol{\sigma} \begin{pmatrix} d_\uparrow \\ d_\downarrow \end{pmatrix}$$

$$S^+ = d_\uparrow^\dagger d_\downarrow \qquad S^- = d_\downarrow^\dagger d_\uparrow \qquad S^z = \frac{1}{2}\left(d_\uparrow^\dagger d_\uparrow - d_\downarrow^\dagger d_\downarrow \right)$$

Exchange interaction

$$\mathbf{S}\cdot\mathbf{s} = S^z s^z + \frac{1}{2}\left(S^+ s^- + S^- s^+\right)$$

spin-preserving scattering

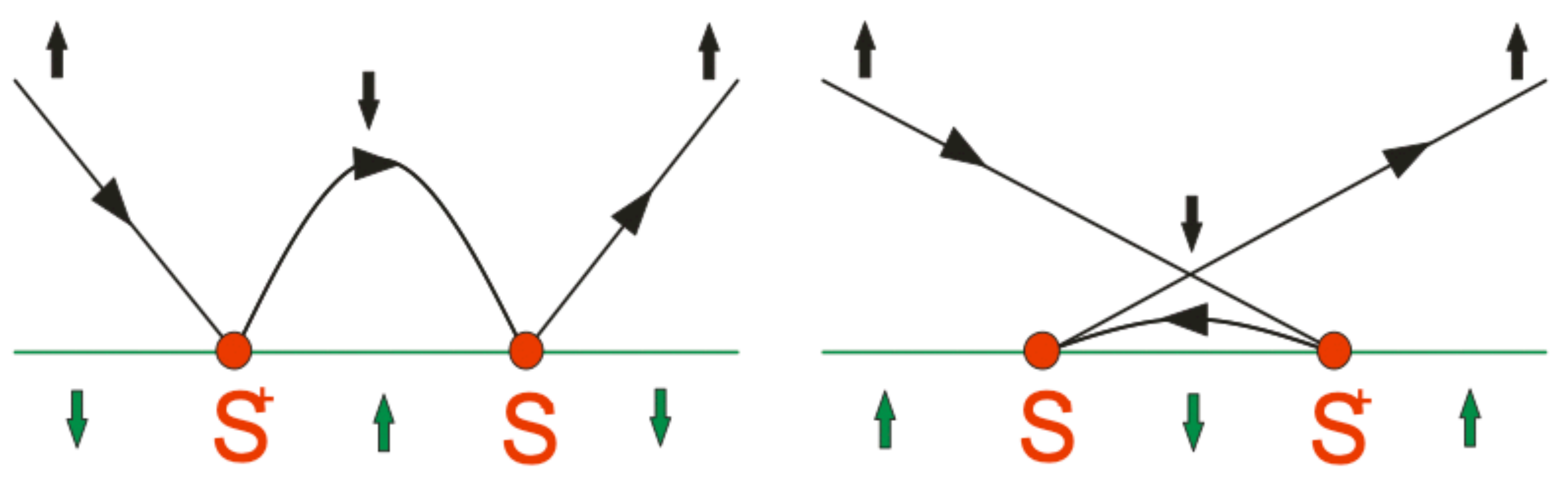
spin-flip scattering

Note: in the large-S limit, the longitudinal part persists, but the spin-flip scattering becomes negligible (1/S correction).

$$S^z|s,s\rangle = s|s,s\rangle$$

vs. $S^-|s,s\rangle = \sqrt{s(s+1)-s(s-1)}|s,s\rangle = \sqrt{2s}|s,s\rangle$

NON-COMMUTATIVE SCATTERING



$$[S_i, S_j] = i\epsilon_{ijk}S_k$$

scattering depends on the previous scattering events, i.e., there are non-trivial temporal <u>correlations</u>

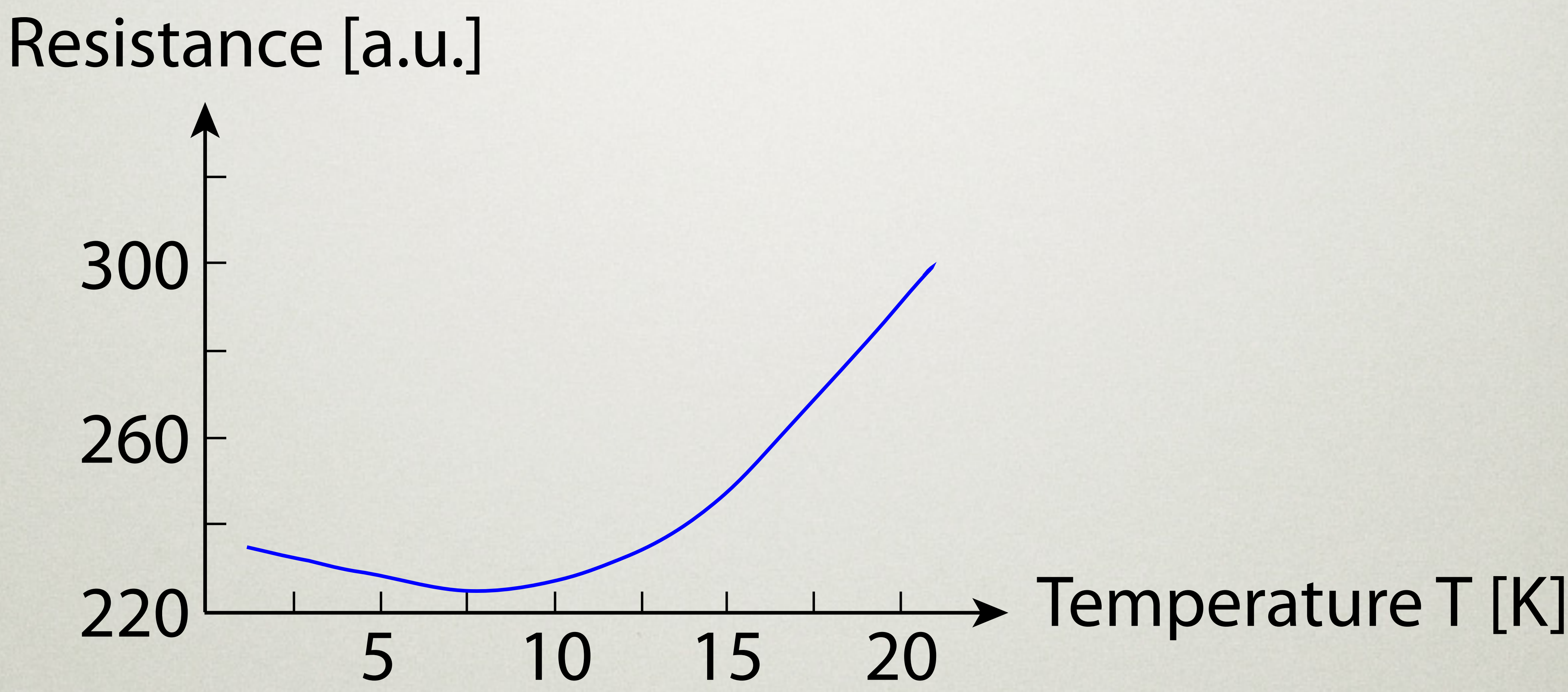
$$(4J^3/N^3)\sum_n M_n{}^2 \sum_{\mathbf{q}} f^0{}_{\mathbf{q}}/(\varepsilon_{\mathbf{q}}-\varepsilon_{\mathbf{k}}). \tag{7}$$

This term has remained because of the difference of matrix elements between the process 3 and 4. In the third process we first increase the z-component of a localized spin and then decrease it, whereas in the fourth we first decrease it and then increase it. The two processes do not give the same answer, which means $S_+S_- - S_-S_+ \neq 0$. This simply expresses the dynamical character of the localized spin system. It has the internal degrees of freedom.

Kondo (1964)

Magnetic impurities in metal hosts

Low-temperature resistance of Au



resistance minimum at <u>finite</u> temperature

Minimum depends on impurity concentration.

W. J. de Haas and G. J. van den Berg, Physica **3**, 440 (1936)

Impurity contribution to ...

How does the impurity change the properties of the system?

$$\langle o \rangle_{\mathrm{imp}} = \langle o \rangle - \langle o \rangle_0$$

System with impurity

Clean system

$$\langle O \rangle = \langle O \rangle_0 + Nc\langle o \rangle_{\mathrm{imp}} + \mathcal{O}(Nc^2)$$

This is known as the “dilute limit”.

NON-PERTURBATIVE BEHAVIOR

$$H' = -\boldsymbol{\mu} \cdot \mathbf{B} = g\mu_B S_z B$$

$$M_{\text{imp}} = g\mu_B \left(\langle S_z + S_{z,\text{band}} \rangle - \langle S_{z,\text{band}} \rangle_0 \right)$$

$$\chi_{\text{imp}}(T) = \frac{(g\mu_B)^2}{k_B T} \frac{1}{4} \left[1 - \rho J + (\rho J)^2 \ln(k_B T/D) + \ldots \right]$$

$$R(T) = aT^5 + c_{\text{imp}} R_0 - c_{\text{imp}} R_1 \ln\left(\frac{k_B T}{D} \right)$$

Kondo (1964)

Resummation to infinite order does not remove the divergence.

$$g(\varepsilon) = (1/N)\sum_{\mathbf{q}} f^0{}_{\mathbf{q}}/(\varepsilon_{\mathbf{q}} - \varepsilon)$$

We shall investigate the dependence of (9) and (12) on the energy of the initial state, $\varepsilon_{\mathbf{k}}$, which is entirely involved in the function $g(\varepsilon_{\mathbf{k}})$. At the absolute zero of temperature, $f^0{}_{\mathbf{q}}$ can be replaced by a step function, which is unity when $q<k_0$ and zero when $q>k_0$, where k_0 is the magnitude of the Fermi momentum. Then assuming that $\varepsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$, we obtain

$$g(\varepsilon_{\mathbf{k}}) = (3z/2\varepsilon_F)\{1 + (k/2k_0)\log|(k-k_0)/(k+k_0)|\} \quad T=0, \tag{13}$$

where z is the number of conduction electrons per atom. The singular nature of this function is common to the problems concerning the Fermi surface and reflects its sharpness. From this expression and (9) and (12), we see that W increases when the electron approaches the Fermi surface, provided J is negative. Since at $T\neq 0$ the average of $|k-k_0|$ for thermally excited electrons is proportional to T, we can, even at this stage of calculation, expect a term proportional to $\log T$ in the expression of the resistivity.

Kondo problem

Perturbation theory breaks down for arbitrarily small J at low enough temperatures.

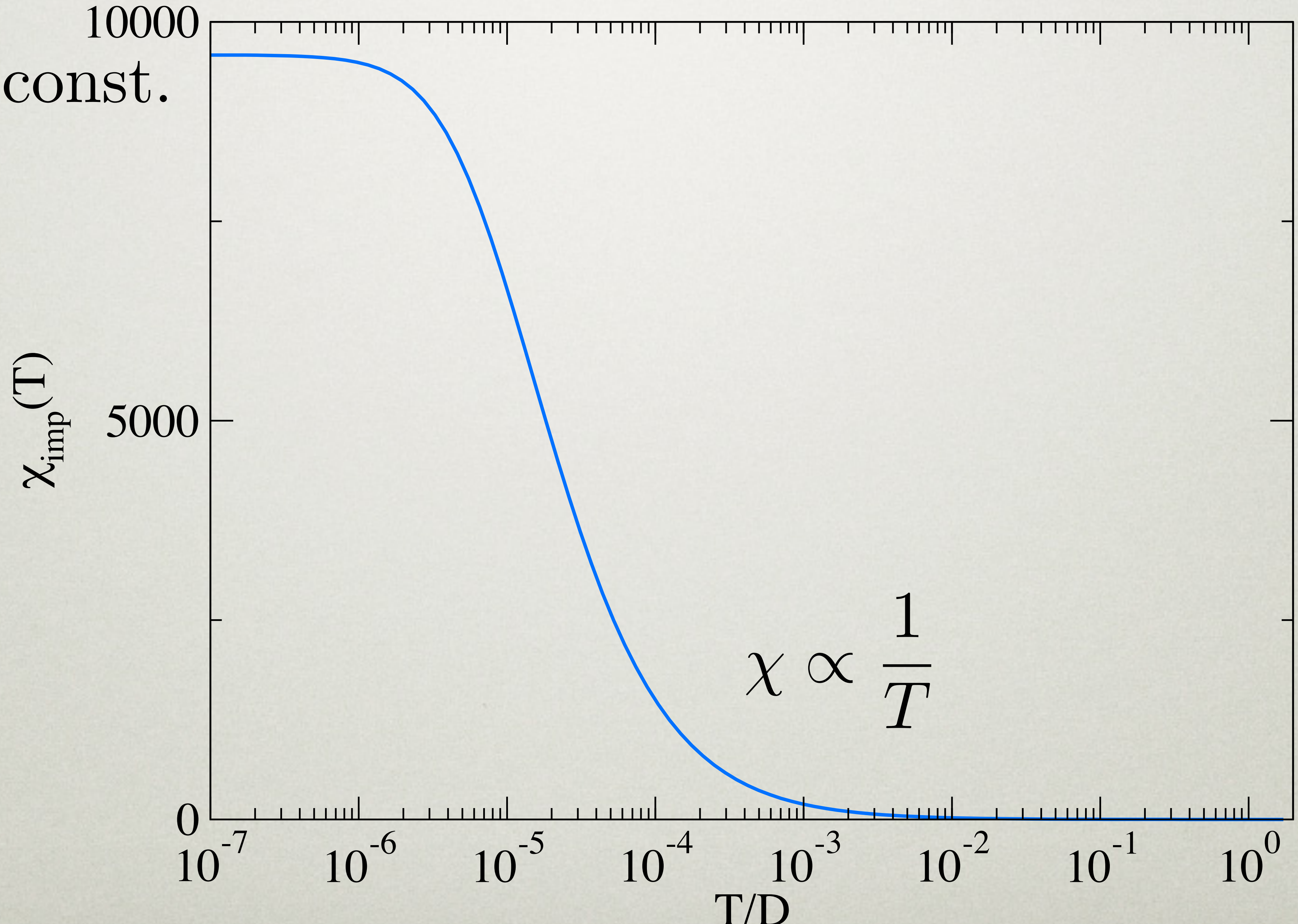
$$k_B T_K \sim D e^{-1/\rho J}$$

Kondo temperature

The Kondo problem: finding a solution valid in the low-temperature $T<T_K$ regime.

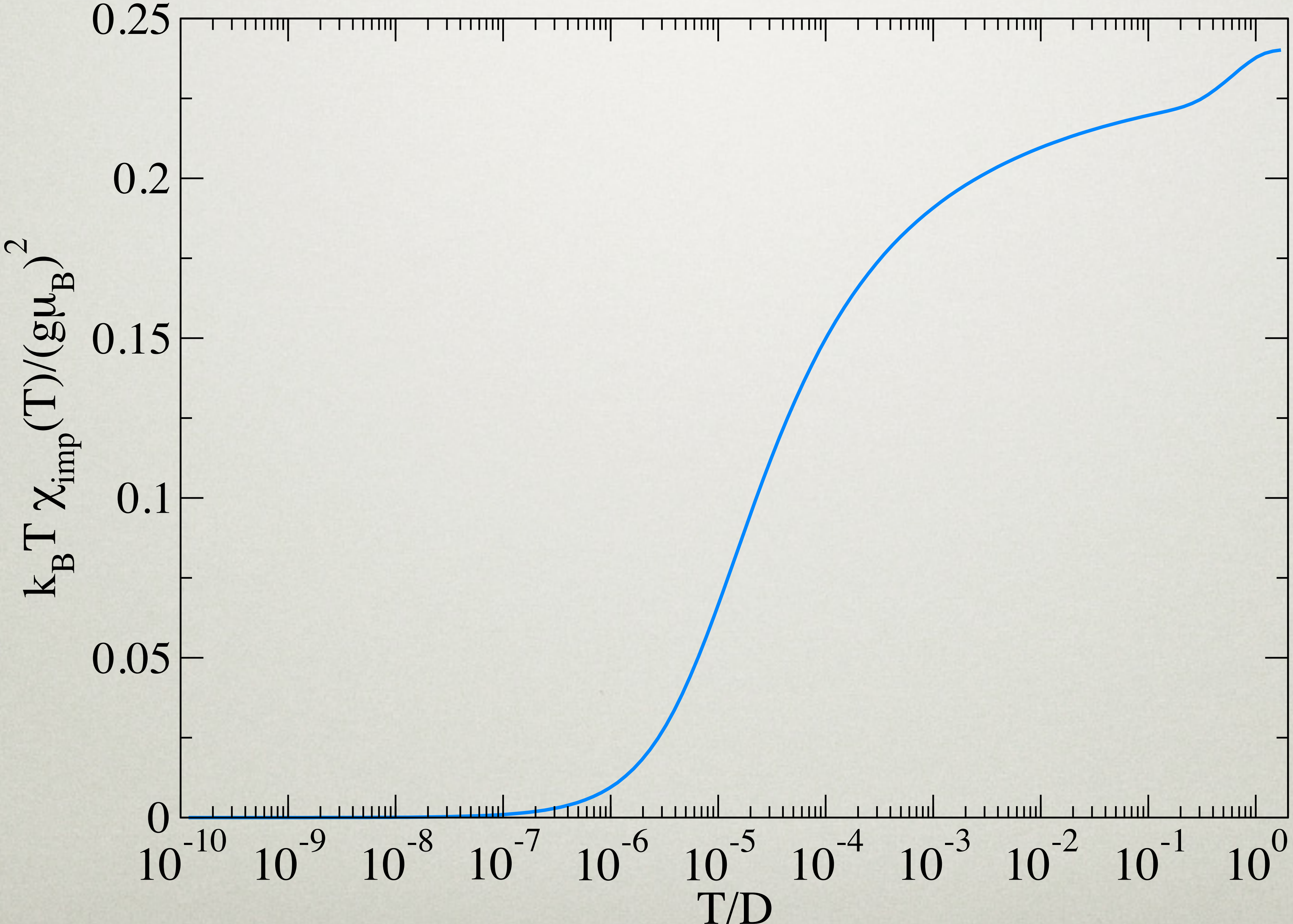
Saturation of impurity susceptibility

$$\chi \propto \frac{1}{T_K} = \text{const.}$$

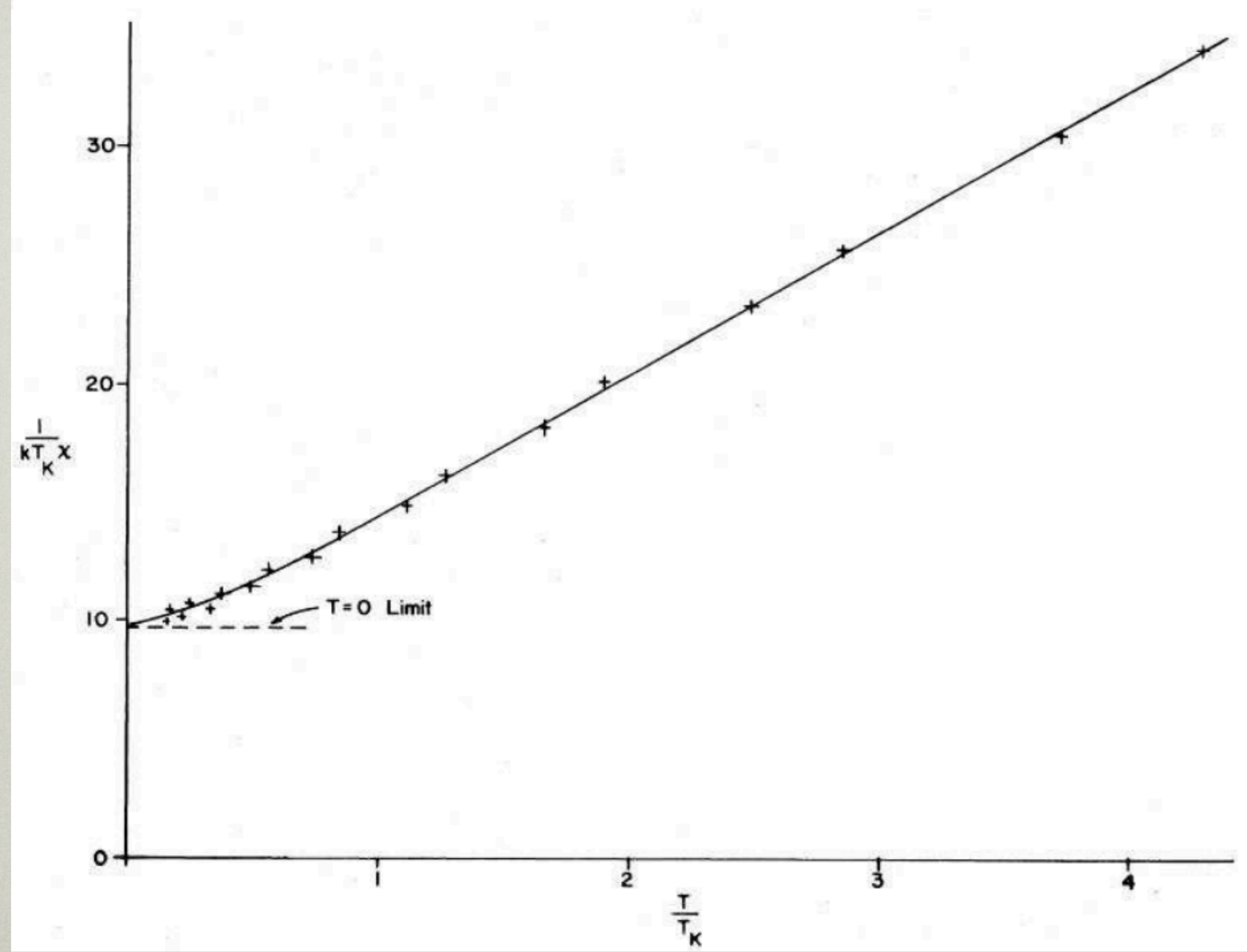


(results of a NRG calculation)

Screening of the local moment

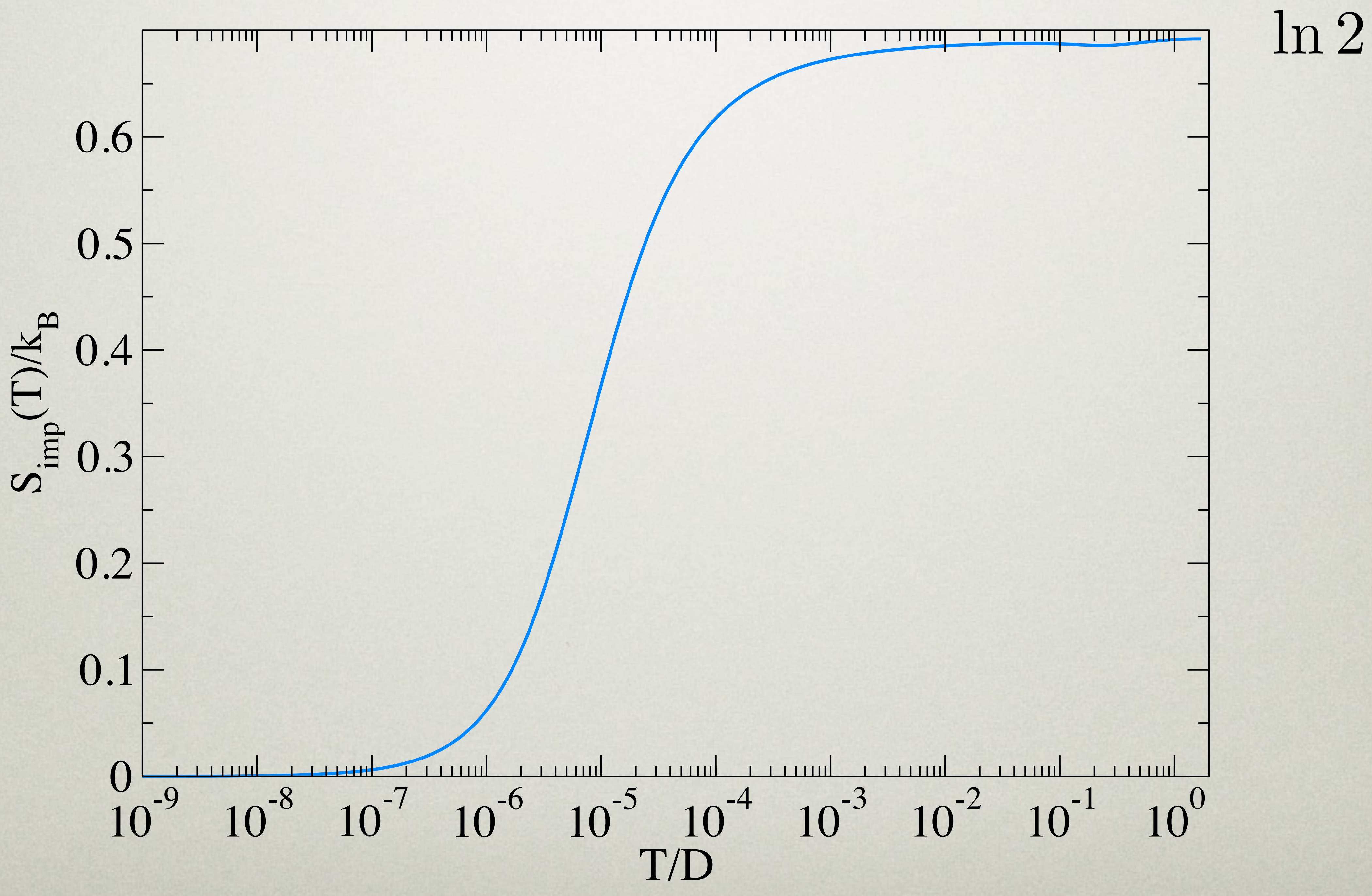


This implies the ground state is a **spin singlet**.

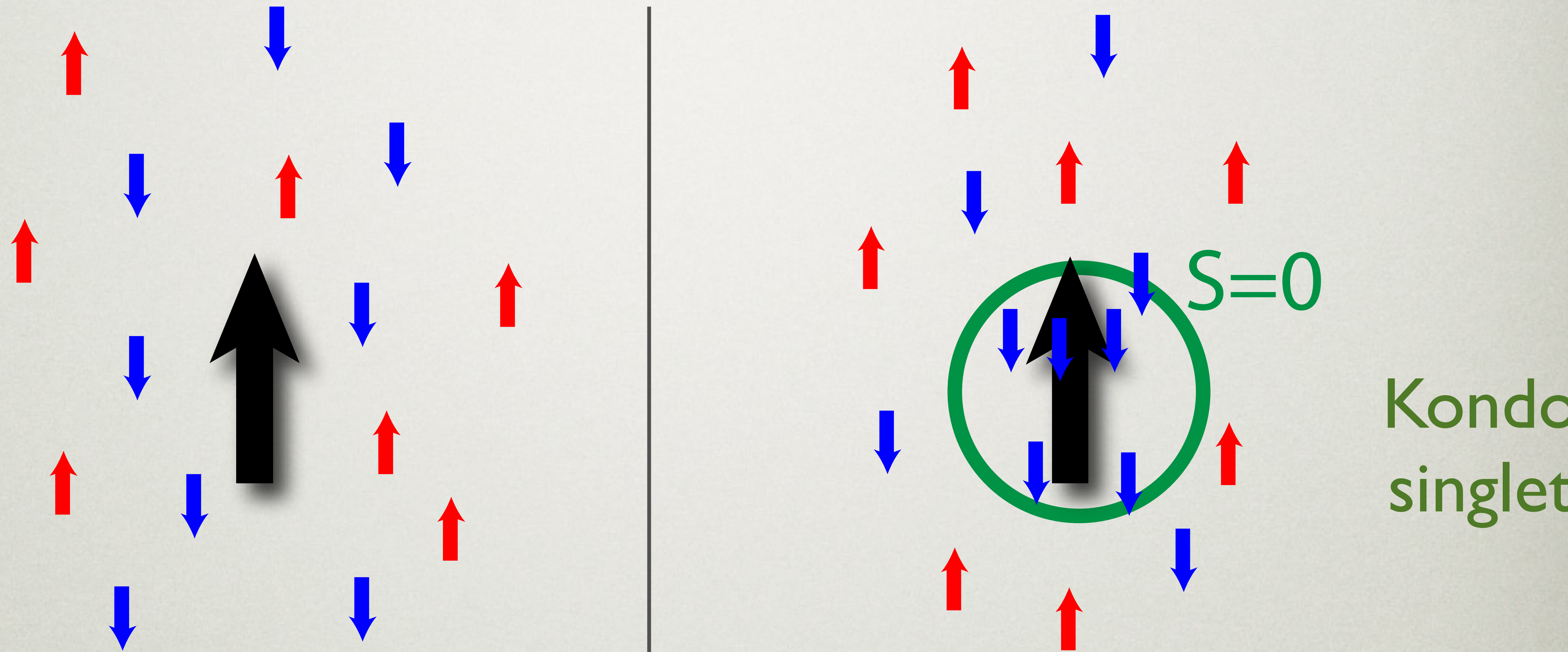


30
20
10
0
$\frac{1}{kT_K}\chi$
T=0 Limit
1
2
3
4
$\frac{T}{T_K}$

Reduction of impurity entropy



The Kondo effect



$$T_K = \mathcal{D} \exp\left(-\frac{1}{\rho J}\right)$$

$T \gg T_K$

free local moments

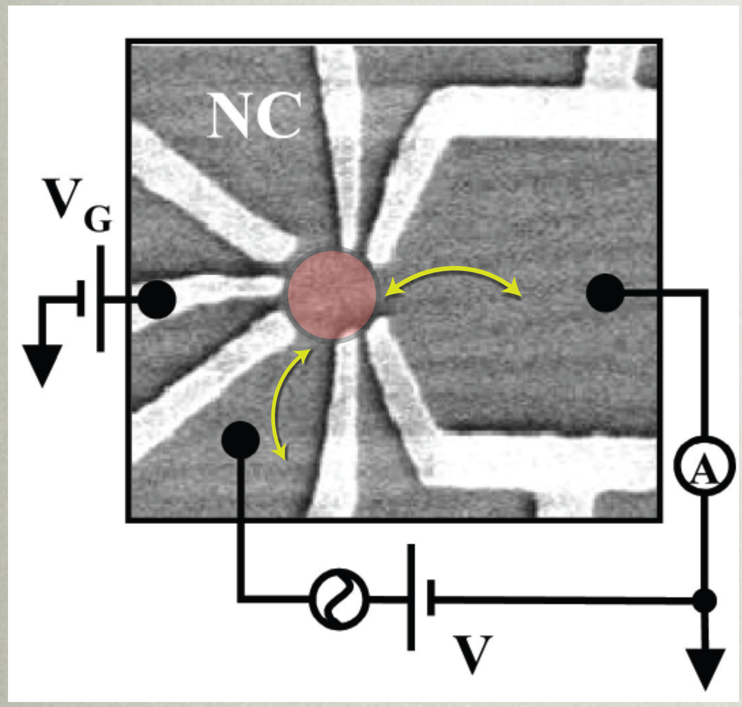
"asymptotic freedom"

$T \ll T_K$

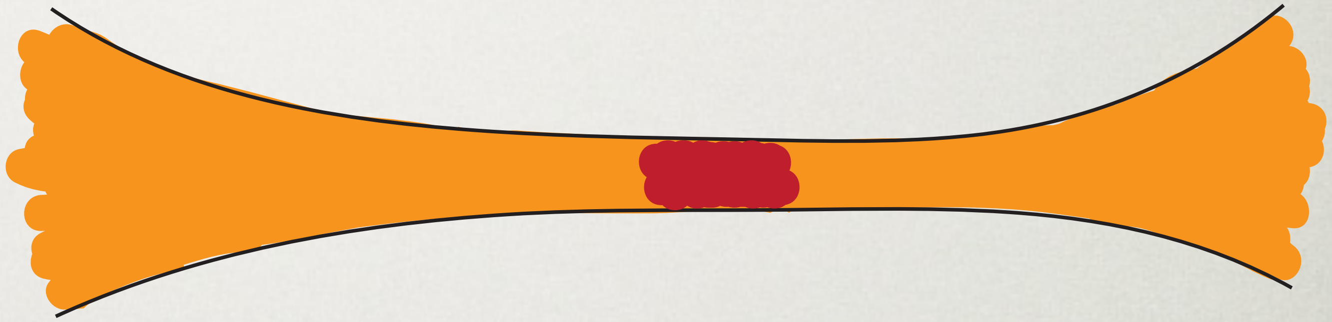
screened local moments

"infrared slavery"

Transport in nanostructures



Grobis et al., PRL 100, 246601 (2008)



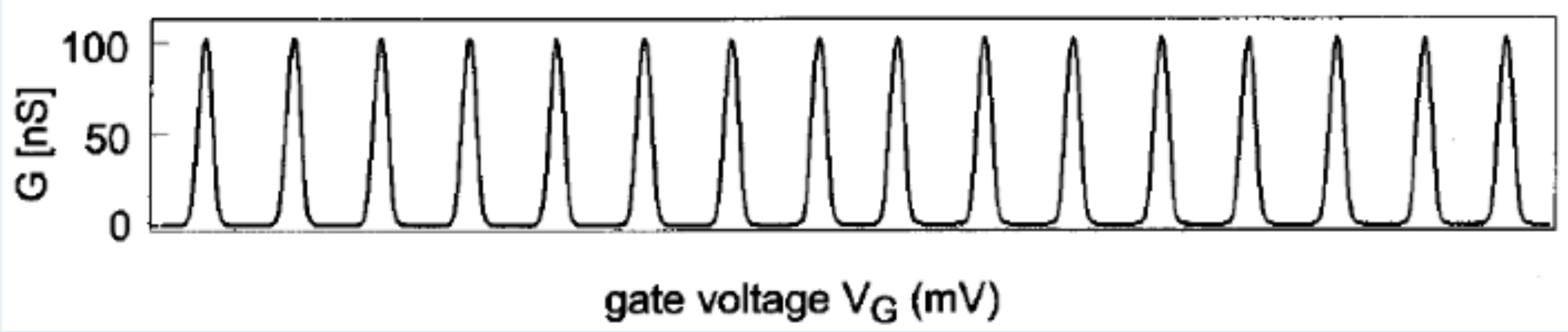
transmission coefficient, T(ϵ)

Landauer formula: $$G = \frac{e^2}{h} \sum_{\sigma} T_{\sigma}(E_F)$$

$$G = \left.\frac{\mathrm{d}I}{\mathrm{d}V}\right|_{V=0}$$

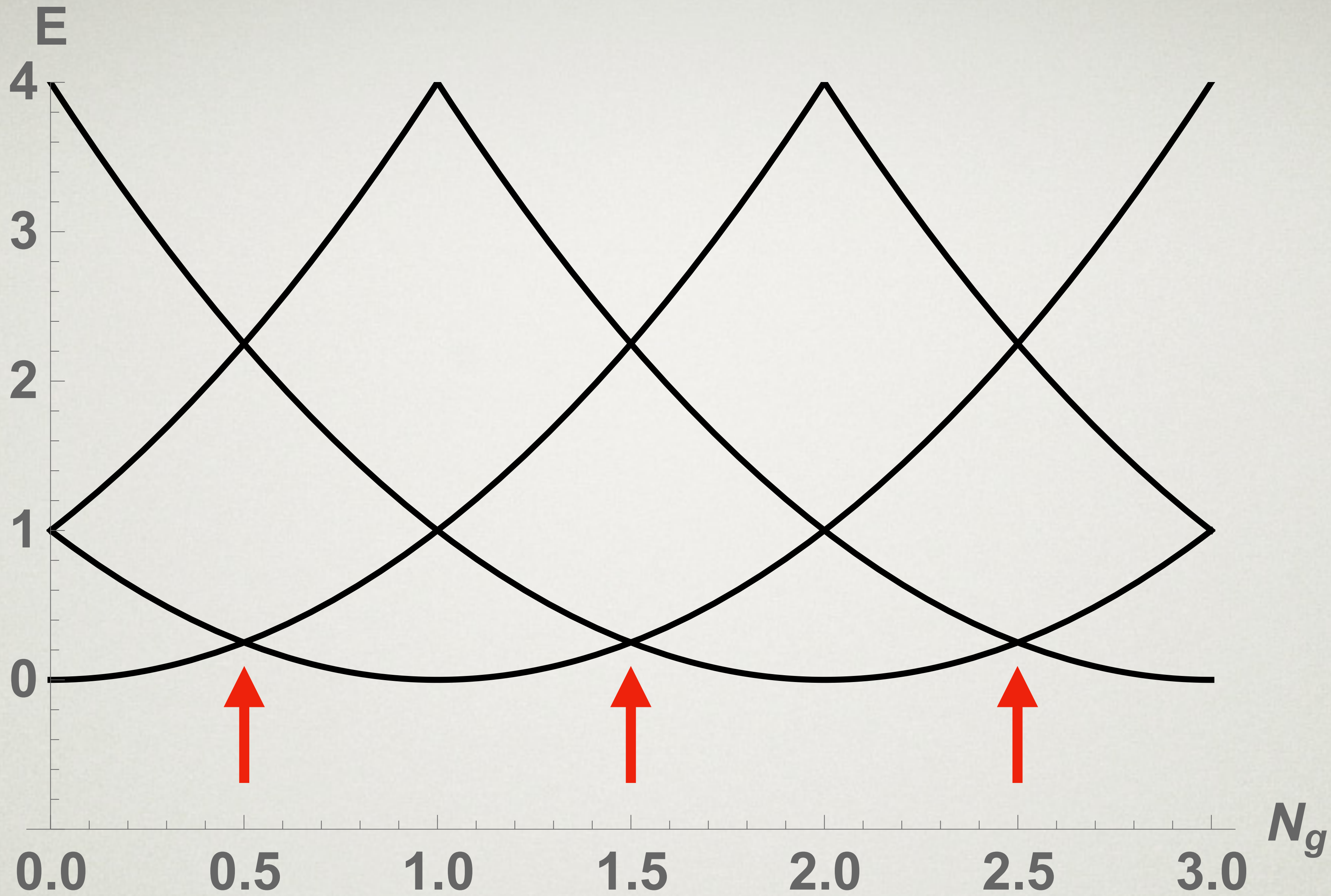
conductance quantum: $$G_0 = \frac{2e^2}{h} = 1/12.906\,\mathrm{k}\Omega$$

Coulomb blockade



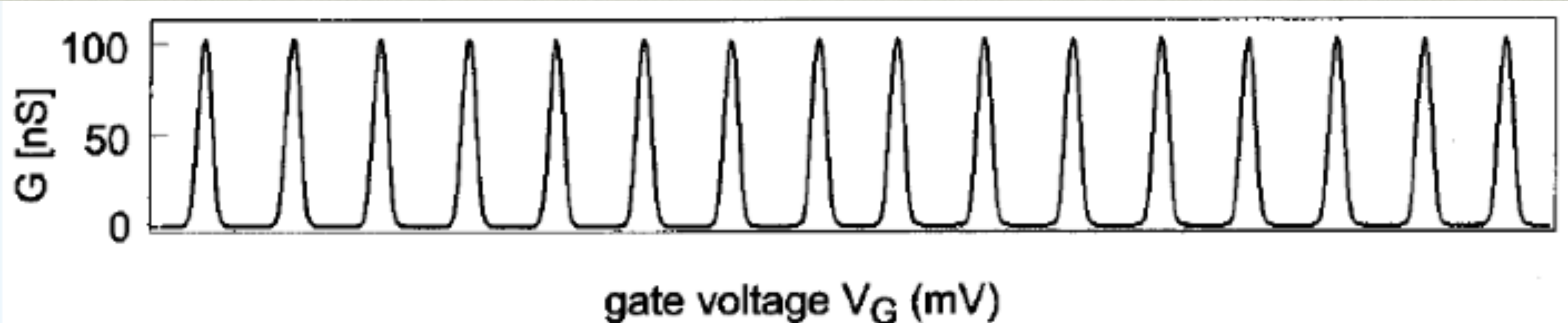
$$E(N, V_g) = UN^2 - \alpha e V_g N = U(N - N_g)^2 + \text{konst.}$$

$$N_g = \frac{\alpha e V_g}{2U}$$

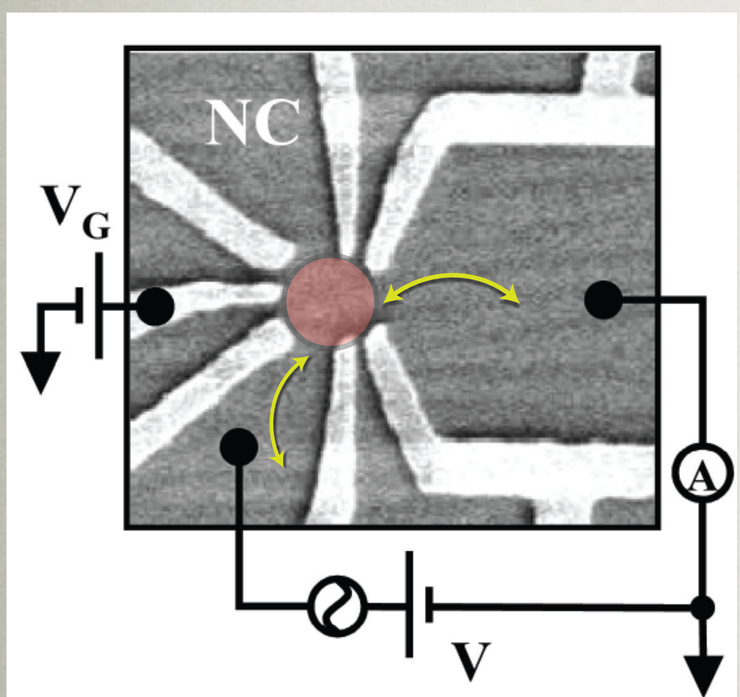


charge degeneracy points:

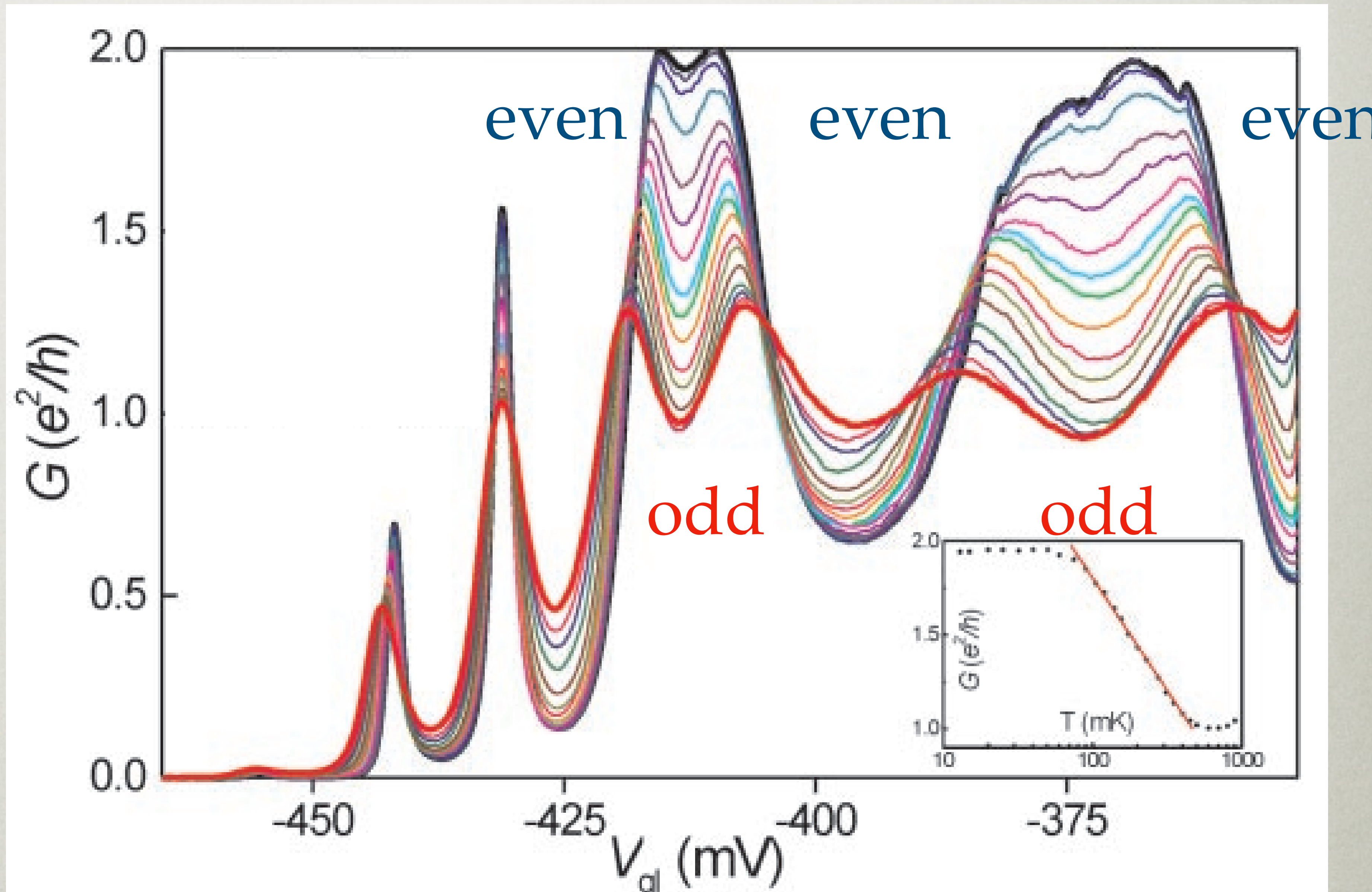
$$E(N+1, V_g) = E(N, V_g) \qquad N_g = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots$$



Kondo effect in quantum dots



Grobis et al., PRL 100, 246601 (2008)



$$G = \left.\frac{\mathrm{d}I}{\mathrm{d}V}\right|_{V=0}$$

unitary conductance: $G=G_0=2e^2/h$

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

Single-Impurity Anderson model

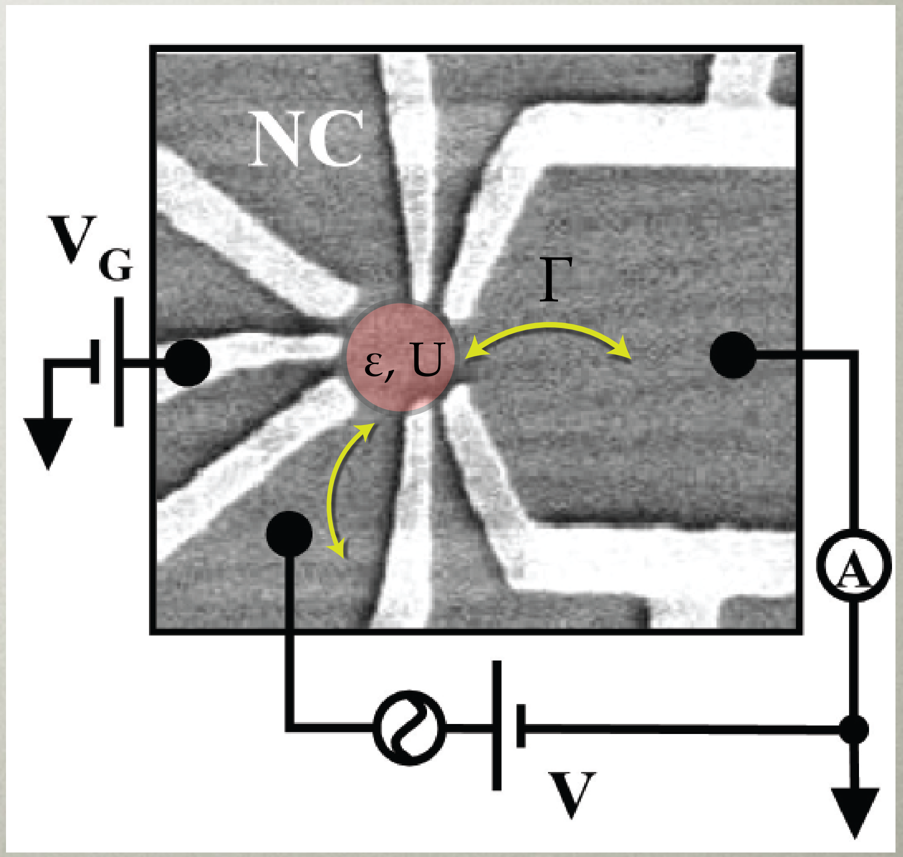
$$H = H_{\text{imp}} + H_{\text{band}} + H_{\text{hyb}}$$

$$H_{\text{imp}} = \sum_{\sigma} \boxed{\epsilon}\, n_\sigma + \boxed{U}\, n_\uparrow n_\downarrow \qquad n_\sigma = d_\sigma^\dagger d_\sigma$$

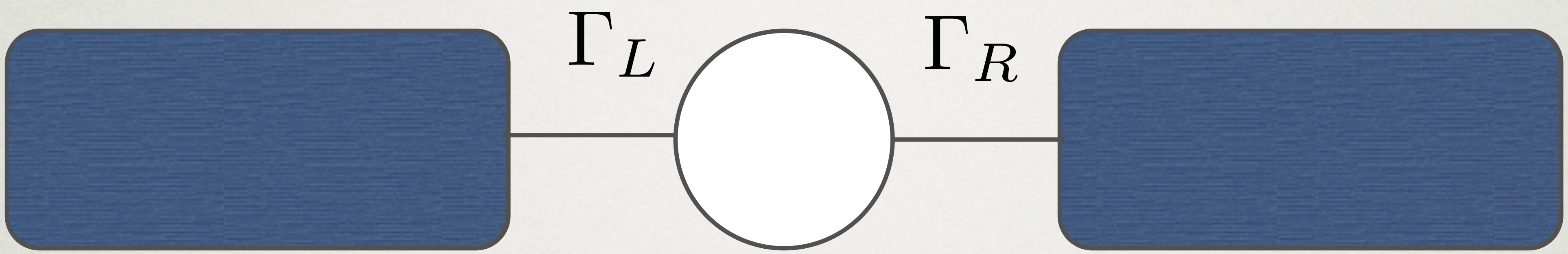
$$H_{\text{band}} = \sum_{\mathbf{k},\sigma} \epsilon_k \, c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma}$$

$$H_{\text{hyb}} = \sum_{k,\sigma} \left(V_k \, c_{k,\sigma}^\dagger d_\sigma + \text{H.c.} \right)$$

$$\Delta(\omega) = \sum_k \frac{|V_k|^2}{\omega - \epsilon_k} \approx i\boxed{\Gamma}$$



Meir-Wingreen formula



$$I = \mathrm{d}/\mathrm{dt}\, N_L = i[H, N_L]$$

$$I = \frac{ie}{2h}\int d\epsilon \left(\mathrm{Tr}\left\{\left[f_L(\epsilon)\mathbf{\Gamma}^L - f_R(\epsilon)\mathbf{\Gamma}^R\right]\left(\mathbf{G}^r - \mathbf{G}^a\right)\right\} + \mathrm{Tr}\left\{\left(\mathbf{\Gamma}^L - \mathbf{\Gamma}^R\right)\mathbf{G}^<\right\}\right)$$

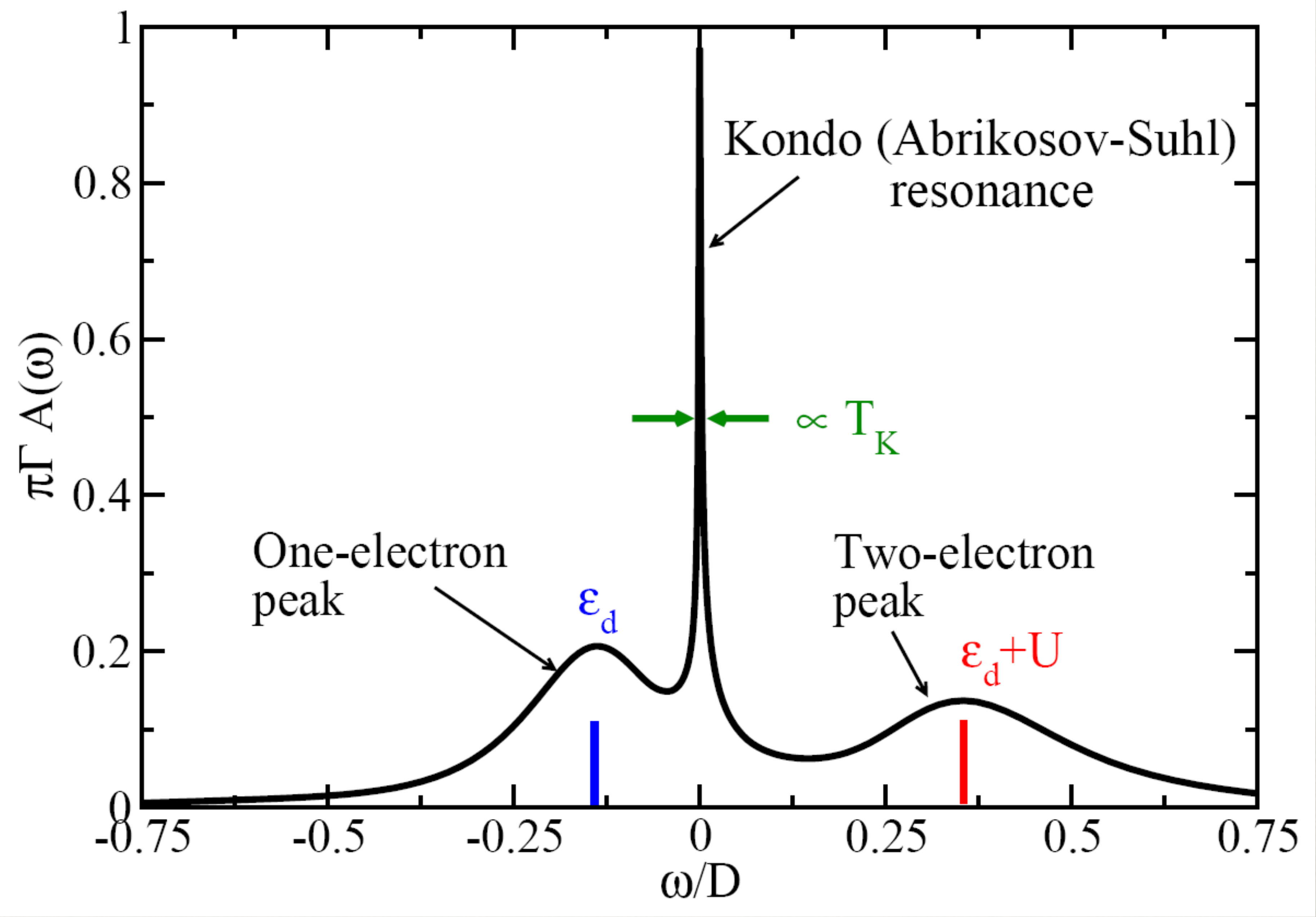
$$G(T) = G_0 \pi\Gamma \int_{-\infty}^{\infty} \mathrm{d}\omega \Big(-\frac{\partial f}{\partial \omega}\Big) A(\omega, T)$$

$$G = G_0 \pi \Gamma A(\omega = 0)$$

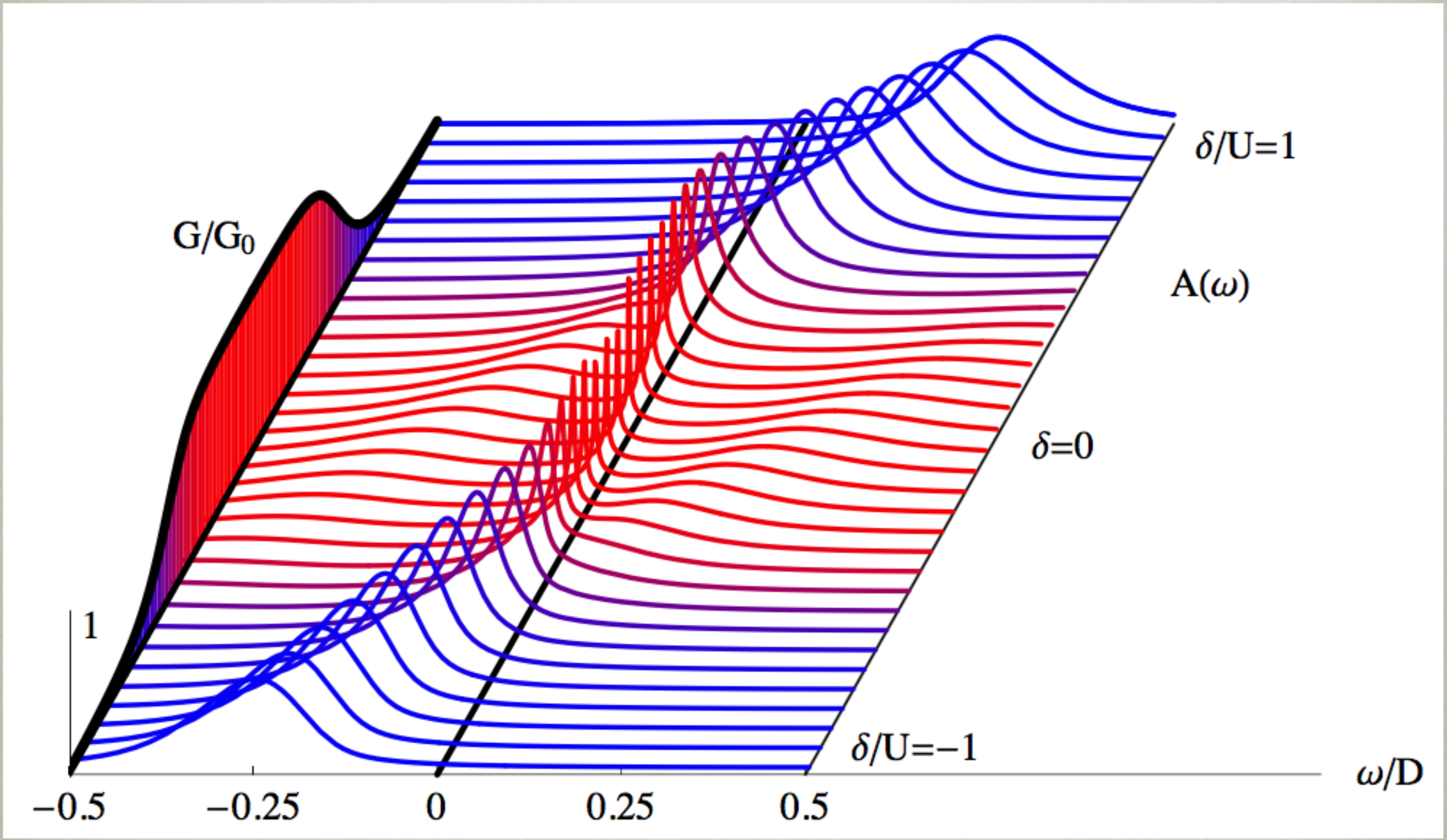
$$f(\omega) = \frac{1}{1 + e^{\beta\omega}}$$

Meir, Wingreen PRL 1992

Kondo resonance



Frota, Oliveira, PRB 33, 7871 (1986), Costi, Hewson, Zlatić, JPCM 6, 2519 (1994)



$$\delta = \epsilon_d + U/2$$

Local Fermi-liquid

phenomenological Fermi liquid theory, Landau 1956
key ideas: Pauli exclusion principle, adiabatic continuity
weakly interacting fermionic quasiparticles
local Fermi liquid for Kondo model, Nozières 1974

$$\delta_\alpha = \pi \langle n_{\mathrm{imp},\alpha} \rangle$$

scattering phase shift for quasiparticles

$\alpha = \uparrow, \downarrow$

$$A_\alpha(\omega = 0) = \frac{1}{\pi \Gamma_\alpha} \sin^2(\delta_\alpha)$$

$G_0 = \frac{2e_0^2}{\hbar}$

$$G_\alpha(0) = G_0 \sin^2(\delta_\alpha)$$

SCATTERING PHASE SHIFT

$$\psi_{l,p}(r) \xrightarrow[r\to\infty]{} e^{i\delta_l(p)} \sin[pr - \frac{1}{2}l\pi + \delta_l(p)]$$ "modulo π ambiguity"

$$\langle E', l', m' | \mathbf{S} | E, l, m \rangle = \delta(E' - E)\delta_{l'l}\delta_{m'm}\mathbf{s}_l(p)$$

S matrix

$$p = \sqrt{2mE} \qquad \mathbf{s}_l(p) = e^{2i\delta_l(p)}$$

$$f_l(p) = \frac{\mathbf{s}_l - 1}{2ip} = \frac{e^{i\delta_l(p)} \sin \delta_l(p)}{p}$$

partial-wave amplitude

$$\sigma = \sum_l \sigma_l(p) \qquad \sigma_l(p) = 4\pi(2l+1)|f_l(p)|^2 = 4\pi(2l+1)\frac{\sin^2 \delta_l(p)}{p^2}$$

cross-section

J. R. Taylor: Scattering theory (1972)

Luttinger's theorem

PHYSICAL REVIEW VOLUME 118, NUMBER 5 JUNE 1, 1960

Ground-State Energy of a Many-Fermion System. II*

J. M. Luttinger
University of Pennsylvania, Philadelphia, Pennsylvania

AND

J. C. Ward
Carnegie Institute of Technology, Pittsburgh, Pennsylvania

(Received January 7, 1960)

The perturbation series for the ground-state energy of a many-fermion system is investigated to arbitrary order for the "isotropic" case. This is the case of over-all spherical symmetry, both in the interaction and in the unperturbed single particle energies. It is shown that for spin one-half fermions the Brueckner-Goldstone perturbation series is valid to all orders in the perturbation. For spins greater than one-half it is in general incorrect even in the isotropic case, unless the interactions are spin independent.

The discussion to arbitrary order in the interaction is carried out by means of a Feynman-like propagator formalism, which is developed in detail.

PHYSICAL REVIEW VOLUME 119, NUMBER 4 AUGUST 15, 1960

Fermi Surface and Some Simple Equilibrium Properties of a System of Interacting Fermions*

J. M. Luttinger†
University of Pennsylvania, Philadelphia, Pennsylvania

(Received March 28, 1960)

It is shown that certain analytical properties of the propagators of many-fermion systems lead rigorously to the existence of sharp discontinuities of the momentum distribution at absolute zero. This discontinuity in the momentum distribution is used to define a Fermi surface for a system of interacting fermions. It is shown that the volume of this surface in momentum space is unaffected by the interaction. The same analytic properties are shown to lead, by direct statistical mechanical arguments, to simple expressions for the low-temperature heat capacity, the spin paramagnetism, and the compressibility of the system. These expressions are very analogous to the corresponding expressions for noninteracting particles. Finally, it is shown how the whole formalism may be generalized when an external periodic potential is present (band case).

Particle density of interacting fermions is equal to the volume in the momentum space enclosed by the Fermi surface.

Number of quasiparticles is the same as the number of interacting fermions.

$$\bar{N} = -\frac{\partial\Omega}{\partial\mu} = \frac{1}{\beta}\sum_{l}\sum_{r}\left\{\frac{\partial}{\partial\zeta_l}\ln[\epsilon_r + G_r(\zeta_l) - \zeta_l] + S_r'(\zeta_l)\frac{\partial G_r(\zeta_l)}{\partial\zeta_l}\right\}\exp(\zeta_l 0^+). \quad (57)$$

$$\bar{N} = \sum_{\substack{r \\ \mu - \epsilon_r - K_r(\mu) > 0}} 1, \quad (69)$$

$\epsilon_{pF} + K_{pF}(\mu) = \mu,$[11]

made of isotropy in the argument. Therefore we have [from (LW 69)]

$$\bar{N} = \sum_{\mathbf{k}} \theta(\mu - \epsilon_{\mathbf{k}} - K_{\mathbf{k}}(\mu))$$
$$= \frac{V}{(2\pi)^3}\int d\mathbf{k}\, \theta(\mu - \epsilon_{\mathbf{k}} - K_{\mathbf{k}}(\mu)). \quad (31)$$

Since the surface

$$\mu - \epsilon_{\mathbf{k}} - K_{\mathbf{k}}(\mu) = 0,$$

is by definition the FS, we may also write[7] (31) as

$$\bar{N} = V V_{\mathrm{FS}}/(2\pi)^3. \quad (32)$$

From (30) and (32) we have

$$V_{\mathrm{FS}} = V_{\mathrm{FS}}^0, \quad (33)$$

which is the desired theorem. The interaction may deform the FS, but it cannot change its volume. In the isotropic case, where symmetry requires the FS to remain a sphere, its radius must then remain k_F (the Fermi momentum of the unperturbed system).

$$G_\alpha(z) = \frac{1}{z - \epsilon_\alpha - \Sigma_\alpha(z)} \qquad N = -\frac{1}{\pi}\sum_\alpha \int_{-\infty}^{0} \mathrm{Im} G_\alpha^R(\omega) \mathrm{d}\omega \qquad G \to (1-\Sigma')G + \Sigma' G$$

$$N = -\frac{1}{\pi}\sum_\alpha \mathrm{Im} \ln G_\alpha^R(0) + \sum_\alpha I_\alpha \qquad N = \sum_\alpha \left[\frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{\epsilon_\alpha + \mathrm{Re}\Sigma_\alpha^R(0)}{\mathrm{Im}\Sigma_\alpha^R(0)}\right)\right] + \sum_\alpha I_\alpha$$

$$I_\alpha = -\frac{1}{\pi}\int_{-\infty}^{0} \mathrm{Im}\left[\frac{\partial \Sigma_\alpha^R(\omega)}{\partial \omega} G_\alpha^R(\omega)\right] \mathrm{d}\omega$$

No assumption of translation invariance, applies to any system (including disordered ones, single-impurity models, etc.).

$\mathrm{Im}\Sigma_\alpha^R(0) = 0$

Single-particle-like states at the Fermi surface do not decay.

Holds within perturbation theory.

$$N = \sum_\alpha \left[1 - \theta\left(\epsilon_\alpha + \mathrm{Re}\Sigma_\alpha^R(0)\right)\right] + \sum_\alpha I_\alpha$$

$$N = V_{\mathrm{FS}} + I$$

$$V_{\mathrm{FS}} = \sum_{\mathbf{k},\sigma,n} \left[1 - \theta(\epsilon_{\mathbf{k},\sigma,n} + \mathrm{Re}\Sigma_{\mathbf{k},\sigma,n}^R(0)\right]$$

$$I = \sum_{\mathbf{k},\sigma,n} I_{\mathbf{k},\sigma,n}$$

$$\tilde{\epsilon}_\alpha = z_\alpha \left(\epsilon_\alpha + \mathrm{Re}\Sigma_\alpha^R(0)\right)$$

$$z_\alpha = \left[1 - \frac{\partial \mathrm{Re}\Sigma_\alpha^R(\omega)}{\partial \omega}\right]_{\omega=0}^{-1}$$

$$\tilde{\rho}(\epsilon) = \sum_\alpha \delta(\omega - \tilde{\epsilon}_\alpha)$$

$$N = \int_{-\infty}^{0} \tilde{\rho}(\omega)\mathrm{d}\omega + \sum_\alpha I_\alpha$$

Luttinger-Ward integral = 0 ?

$$\int_{-\infty}^{0} \frac{\partial \Sigma_\alpha(\omega)}{\partial \omega} G_\alpha(\omega) \mathrm{d}\omega = 0$$

Proven within perturbation theory. Thus holds for solutions which are adiabatically connected with the non-interacting state.

Friedel (1952): resonant level model $n = \frac{2}{\pi}\sum_l (2l+1)\delta_l(k_F)$

Langer, Ambegaokar (1961): general interacting model $n = \frac{1}{2\pi i}\mathrm{Tr}\ln \mathbf{s}(\mu)$

Langreth (1966): Anderson impurity model

Shiba (1975): multi-orbital Anderson model with orbital-diagonal interaction

$$\delta_\alpha = \frac{\pi}{2} - \arctan\left(\frac{\epsilon_\alpha + \mathrm{Re}\Sigma_\alpha^R(0)}{\Gamma_\alpha}\right)$$

$$n_\alpha = \left[\frac{1}{2} - \frac{1}{\pi}\arctan\left(\frac{\tilde{\epsilon}_\alpha}{\tilde{\Gamma}_\alpha}\right)\right] + I_\alpha$$

$$n_\alpha = \delta_\alpha/\pi + I_\alpha$$

n_α is the “local charge displacement”, “excess electrons”.
In the wide-bind limit, it is equal to the impurity occupancy.

$$A_\alpha(\omega = 0) = \frac{1}{\pi\Gamma_\alpha}\sin^2(\delta_\alpha)$$

$$G_0 = \frac{2e_0^2}{\hbar}$$

$$G_\alpha(0) = G_0 \sin^2(\delta_\alpha)$$

Are all impurity systems Fermi liquids?

Singular Fermi liquids, I_α=1/2, logarithmic corrections at low ω.

Mehta, Borda, Zarand, Andrei, Coleman (2005)
Logan et al. (2009, 2011, 2014)

example: S=1 single-channel Kondo

Non-Fermi liquids: low-energy excitations are <u>not</u> in a 1:1 correspondence with those of the non-interacting system. Anomalous behavior.

Affleck (1990)

example: S=1/2 two-channel Kondo

THE FAMILY OF KONDO IMPURITY MODELS

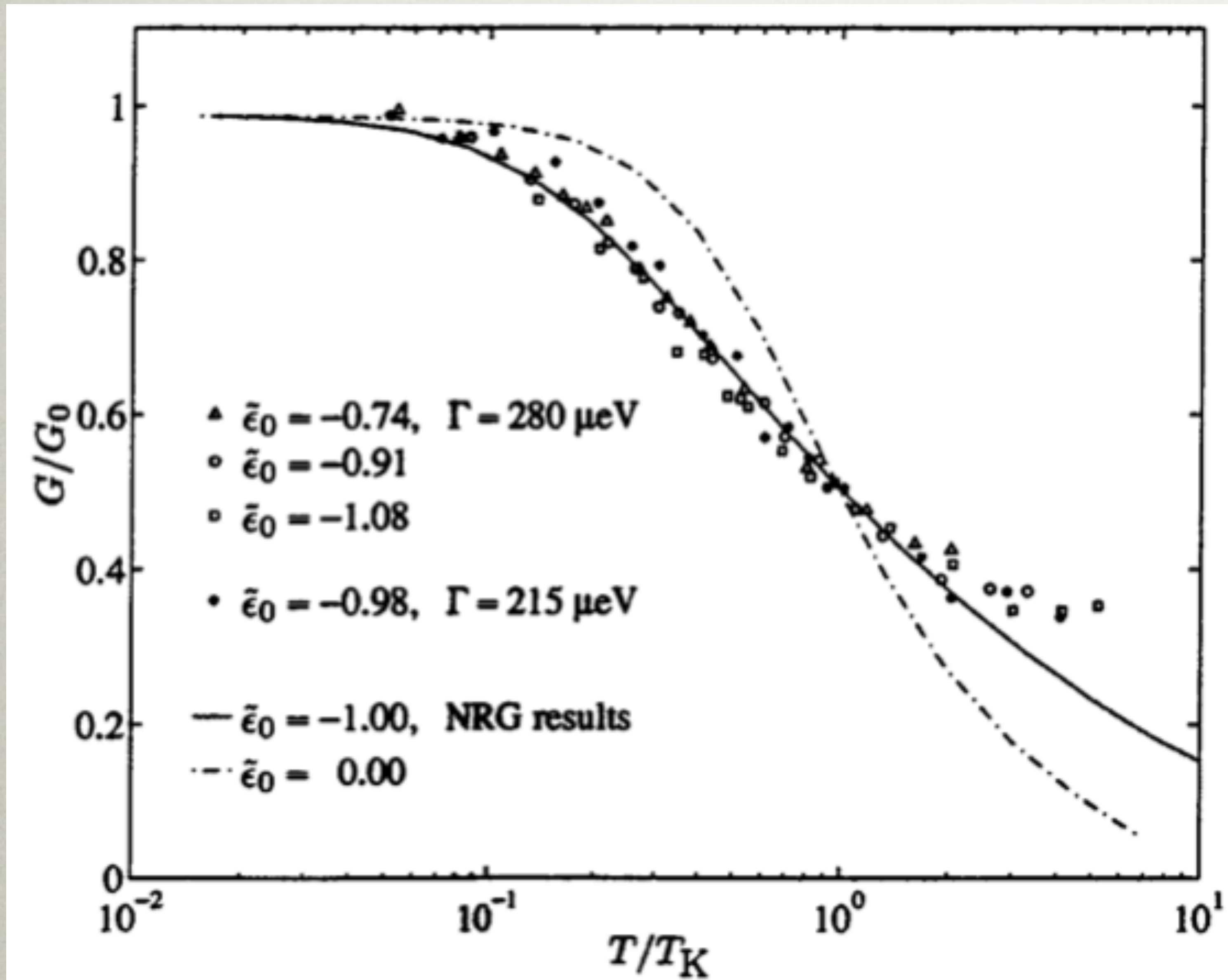
$$H = \sum_{\mathbf{k},\sigma,i} \epsilon_k c^\dagger_{\mathbf{k},\sigma,i} c_{\mathbf{k},\sigma,i} + \sum_i J \mathbf{s}_i \cdot \mathbf{S} + \mathbf{B} \cdot \mathbf{S} \qquad \text{i=1,...,N}_{\text{channels}}$$

Classification according to 2S vs. N_{channels}

	fully screened Kondo model	underscreened Kondo model	overscreened Kondo model
impurity spin, S	1/2	1	1/2
N_{channels}	1	1	2
fixed point	Fermi liquid	singular Fermi liquid	non-Fermi liquid

P. Nozières and A. Blandin. J. Physique 41, 193 (1980)

Standard Kondo effect



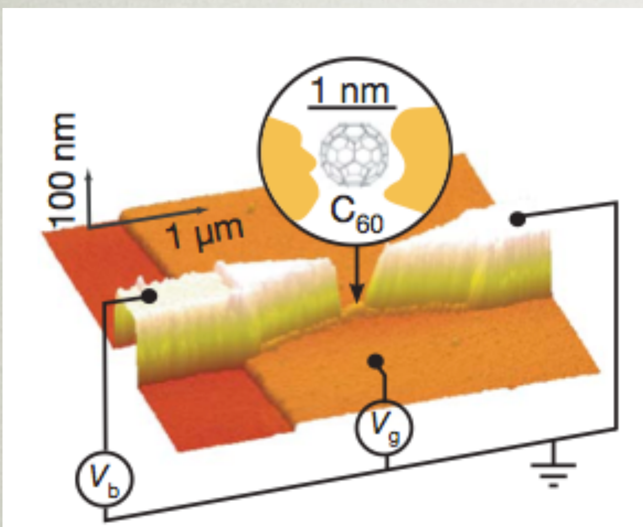
$$G(T_K) = G_0/2$$

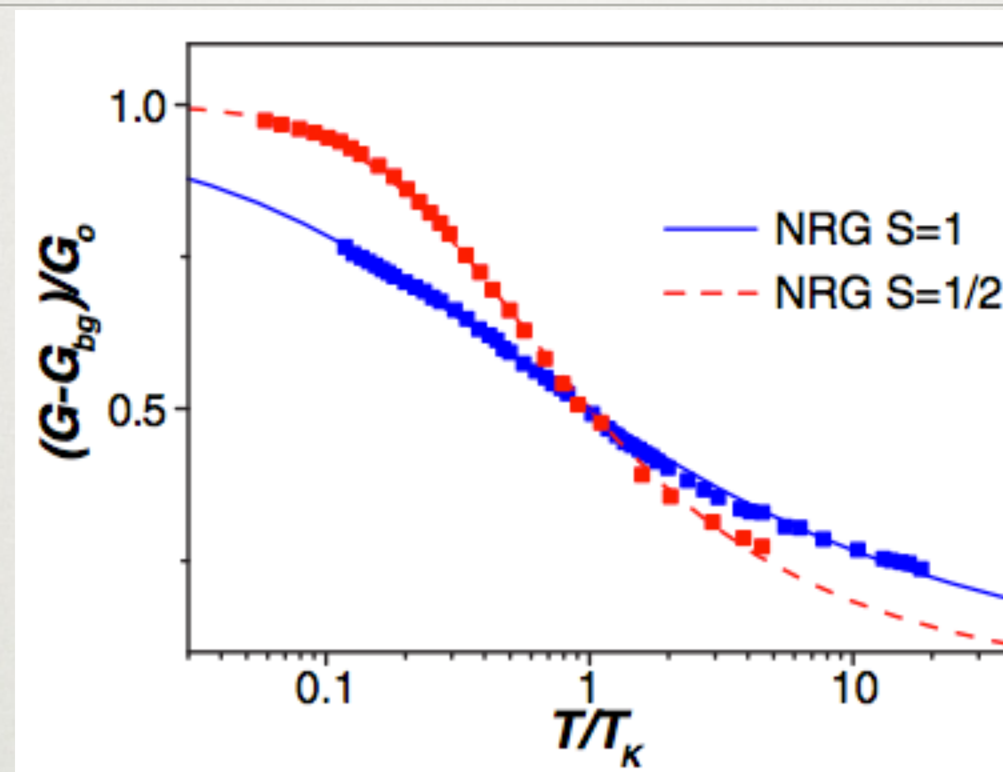
$$G(T) = G_0 \left[1 + (2^{1/s} - 1)(T/T_K)\right]^{-s}$$ s=0.22

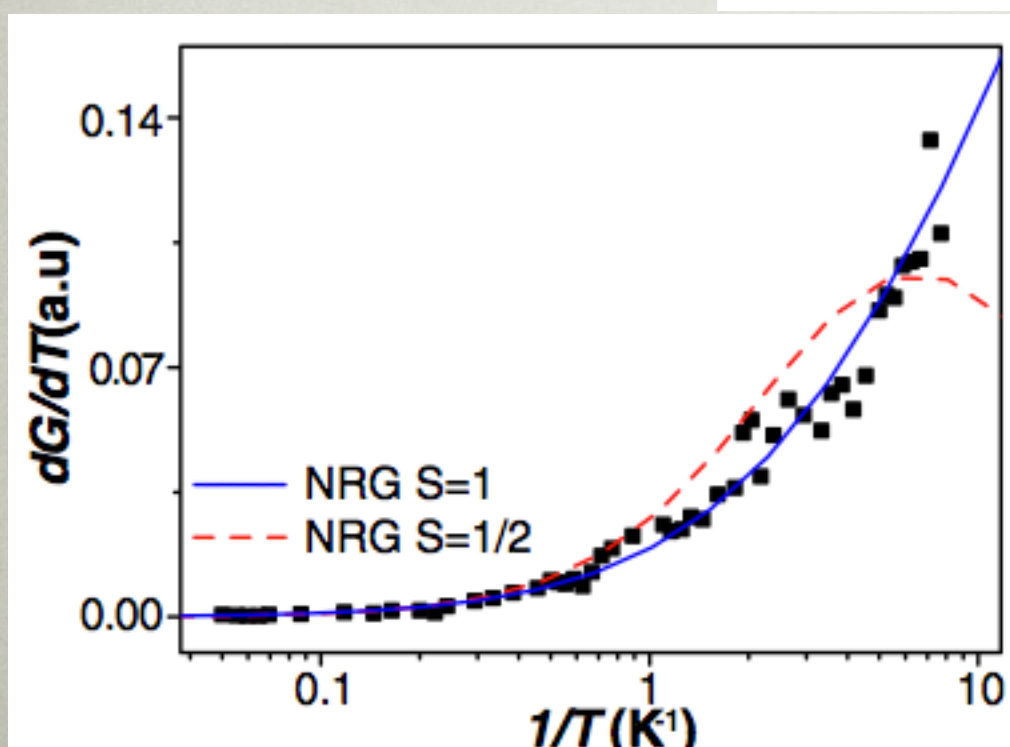
Goldhaber-Gordon et al., Phys. Rev. Lett. 81, 5225 (1998)

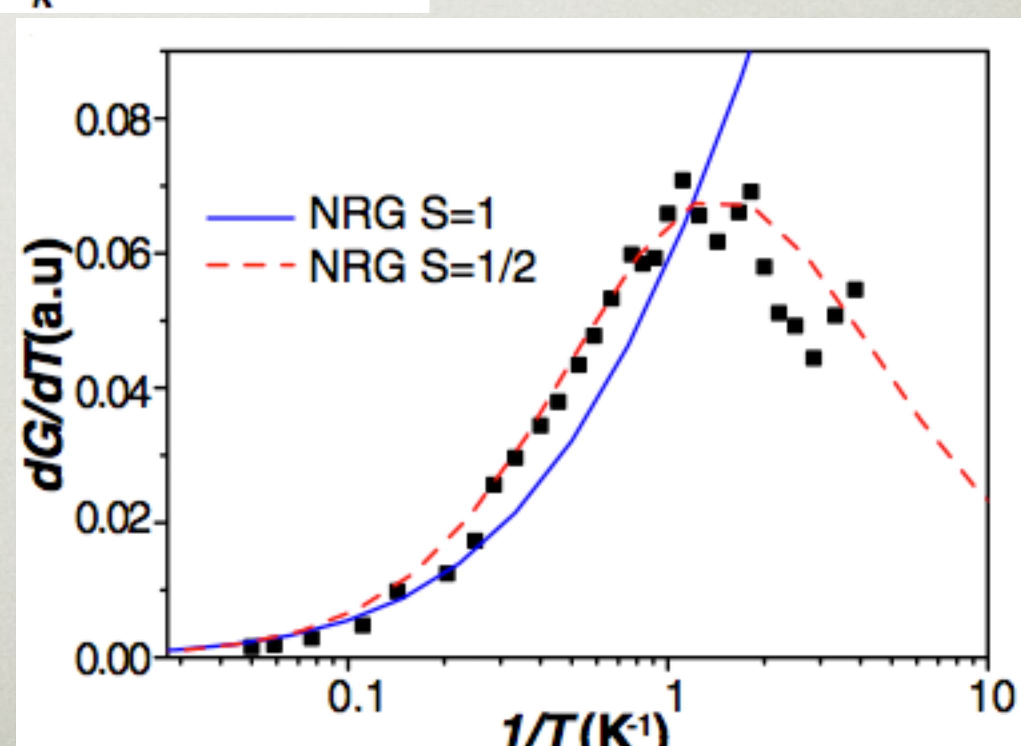
Underscreened Kondo Effect

C_{60} molecule

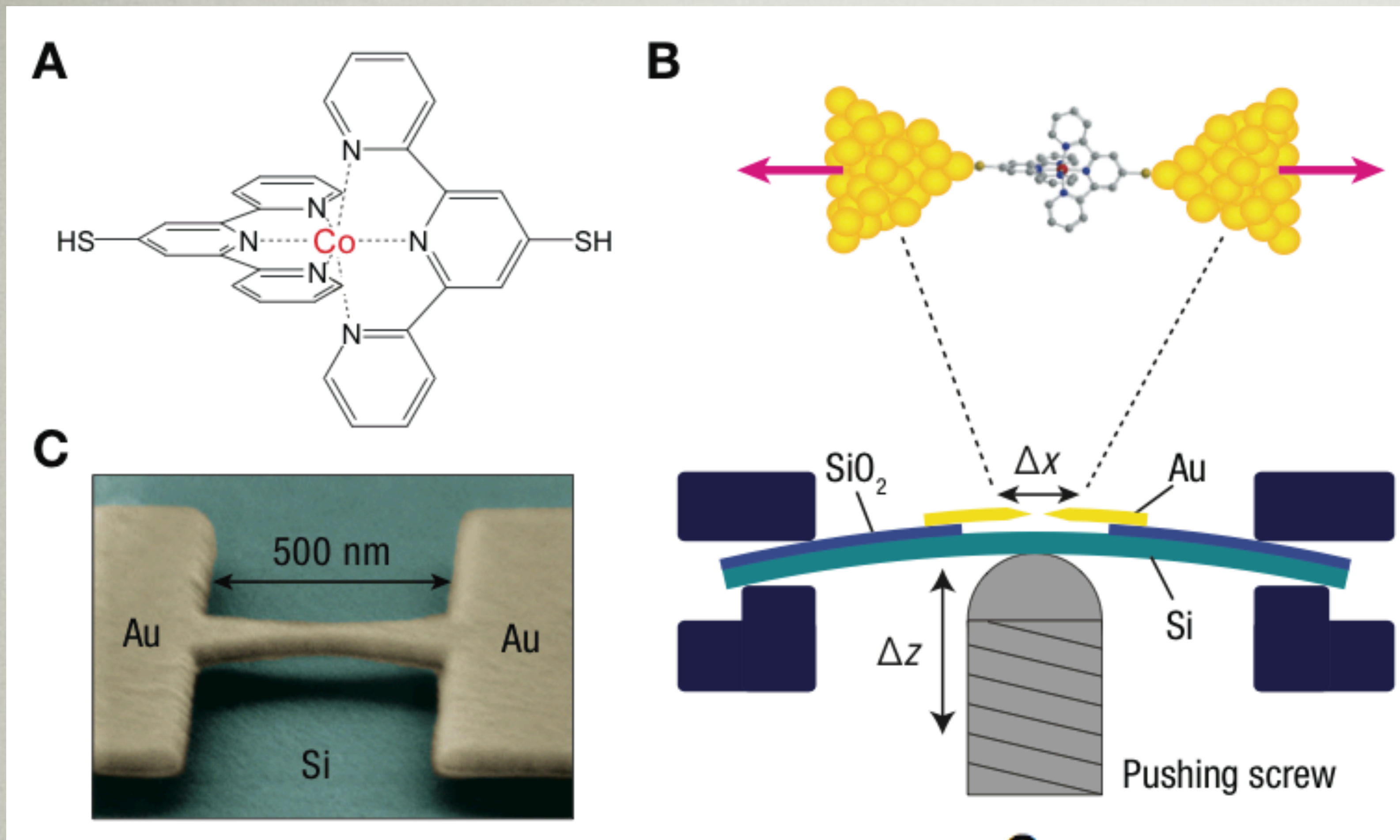


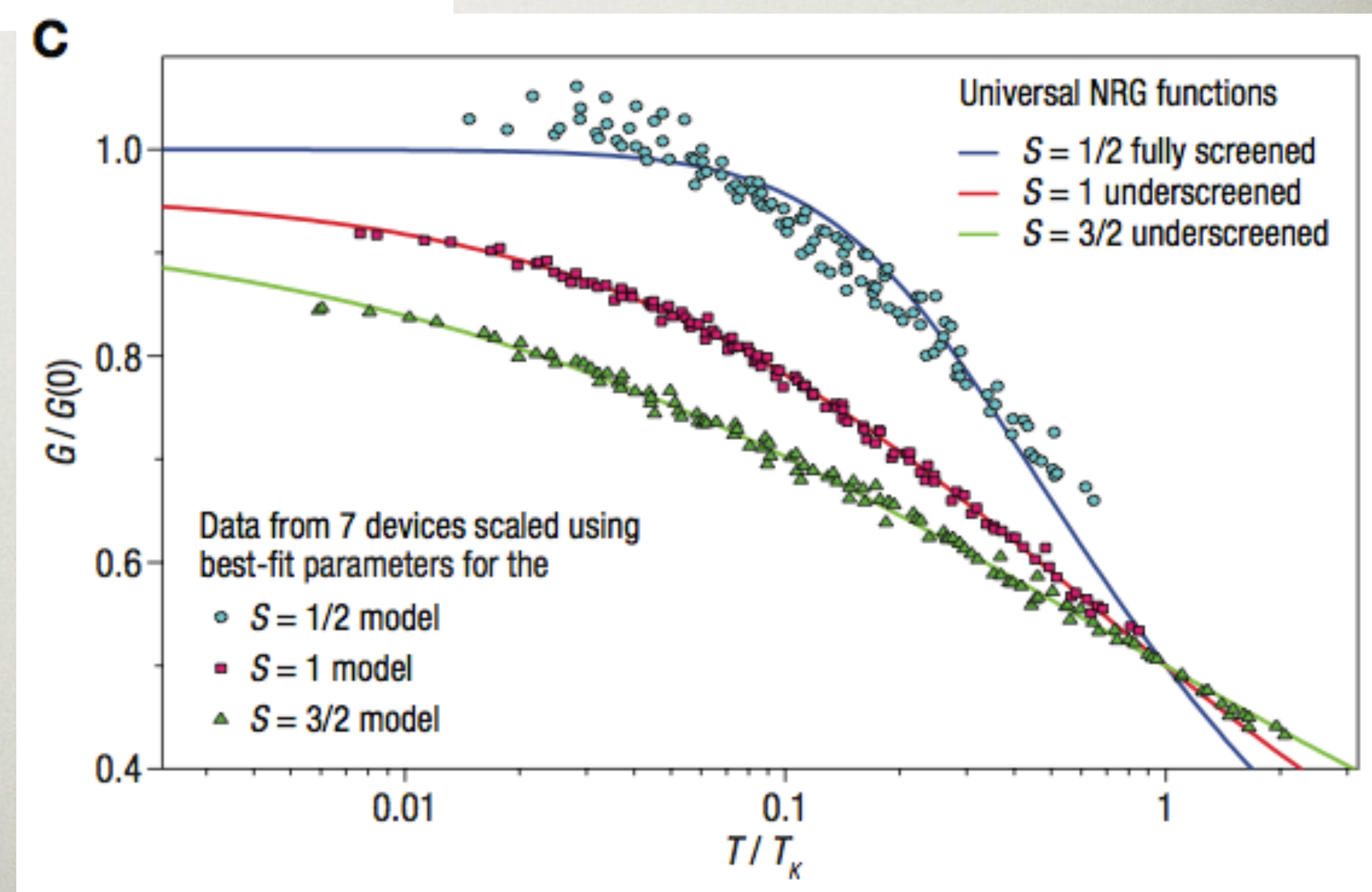






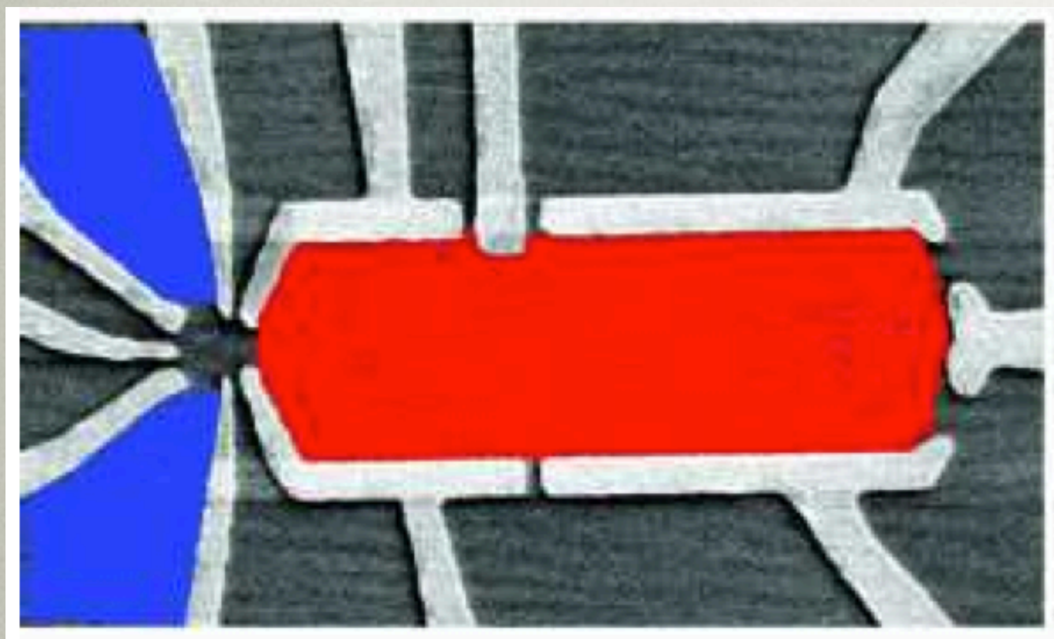
N. Roch, S. Florens, T. A. Costi, W. Wernsdorfer, F. Balestro, PRL 103, 197202 (2009)





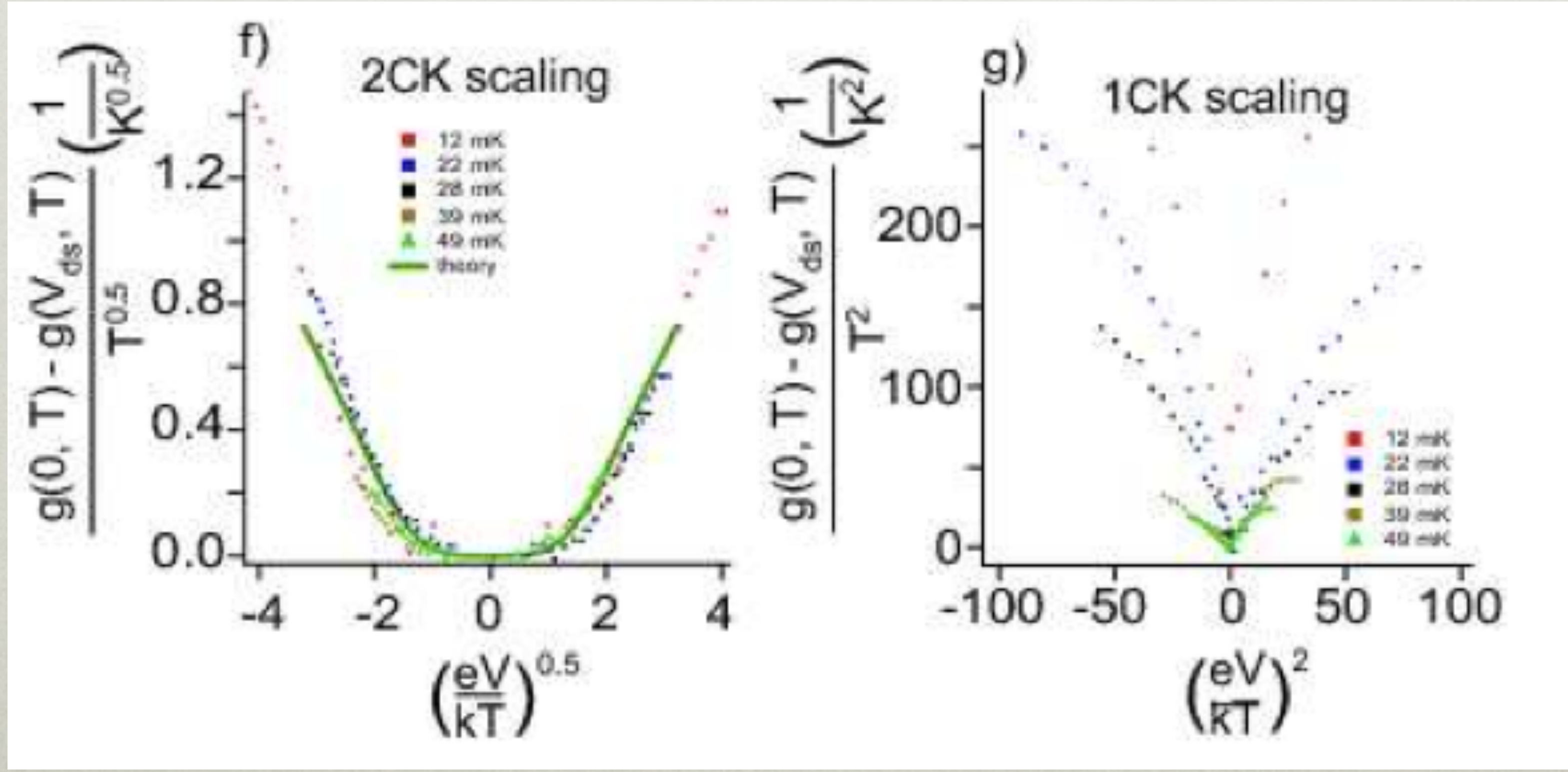
J. J. Parks, A. R. Champagne, T. A. Costi, W. W. Shum, A. N. Pasupathy, E. Neuscamman, S. Flores-Torres, P. S. Cornaglia, A. A. Aligia, C. A. Balseiro, G. K.-L. Chan, H. A. Abruna, and D. C. Ralph. Science 328, 1370 (2010)

Overscreened Kondo effect



$$\frac{g(0,T) - g(V_{\rm sd},T)}{T^{0.5}} \propto Y\left(\frac{eV_{\rm ds}}{k_B T}\right)$$

$$Y(x) \approx \begin{cases} \frac{3}{\pi}\sqrt{x} - 1 & \text{for } x \gg 1 \\ cx^2 & \text{for } x \ll 1 \end{cases}$$

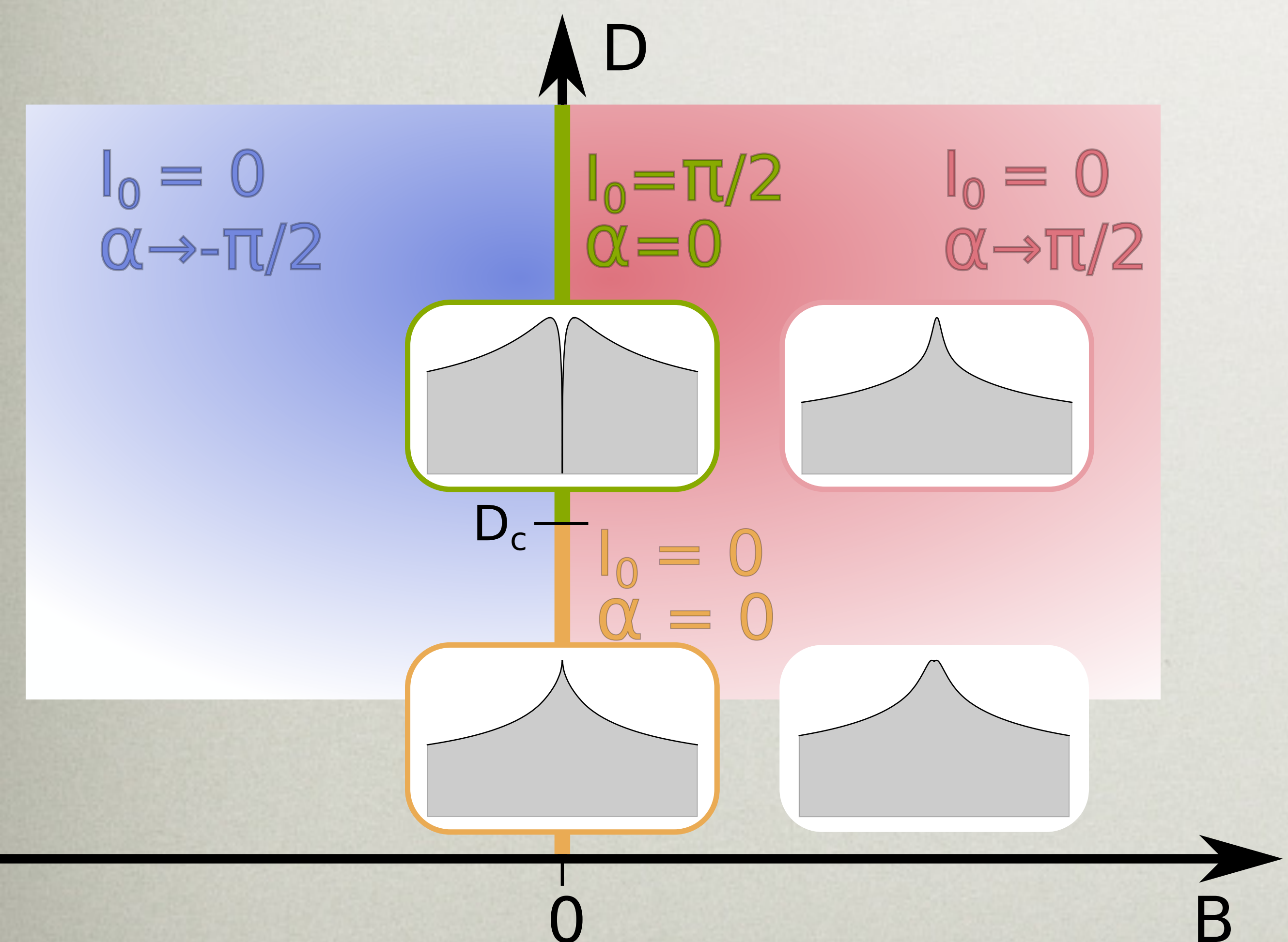


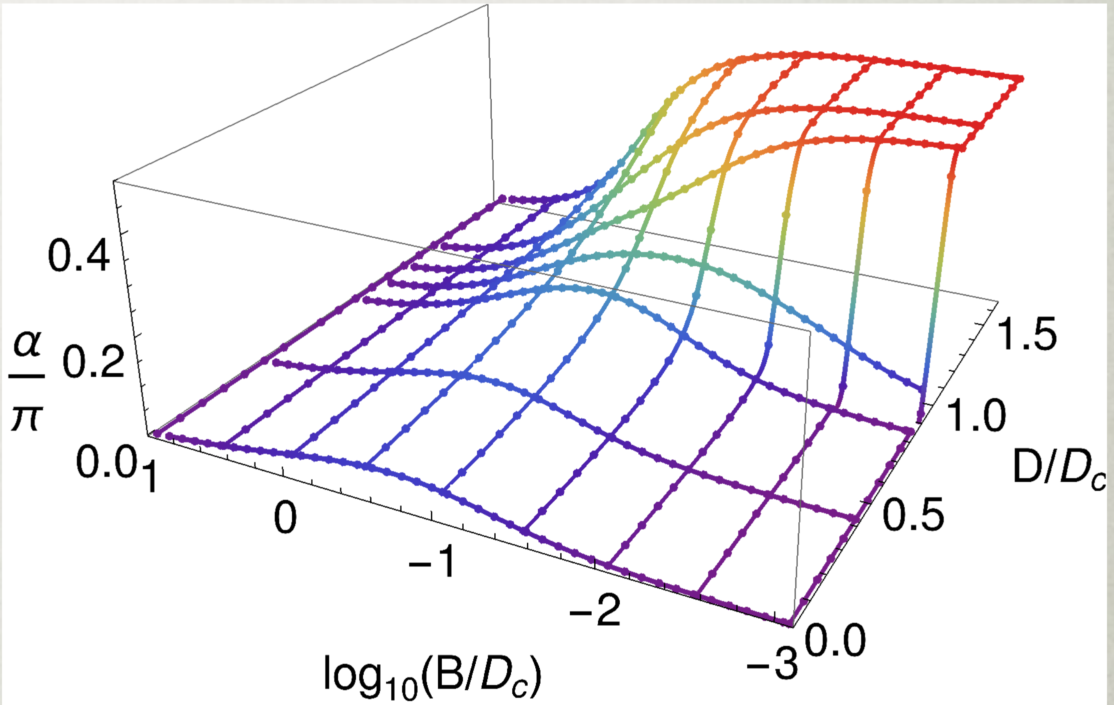
R. M. Potok, I. G. Rau, Hadas Shtrikman, Yuval Oreg, and D. Goldhaber-Gordon, Nature 446, 167 (2007)

Non-Landau Fermi liquid

Regular Fermi liquid but with topological term $I_0=\pi/2$.

$$H = H_{\mathrm{bath}} + J_1 \mathbf{S}\cdot\mathbf{s}_1 + J_2 \mathbf{S}\cdot\mathbf{s}_2 + D S_z^2 + B S_z$$

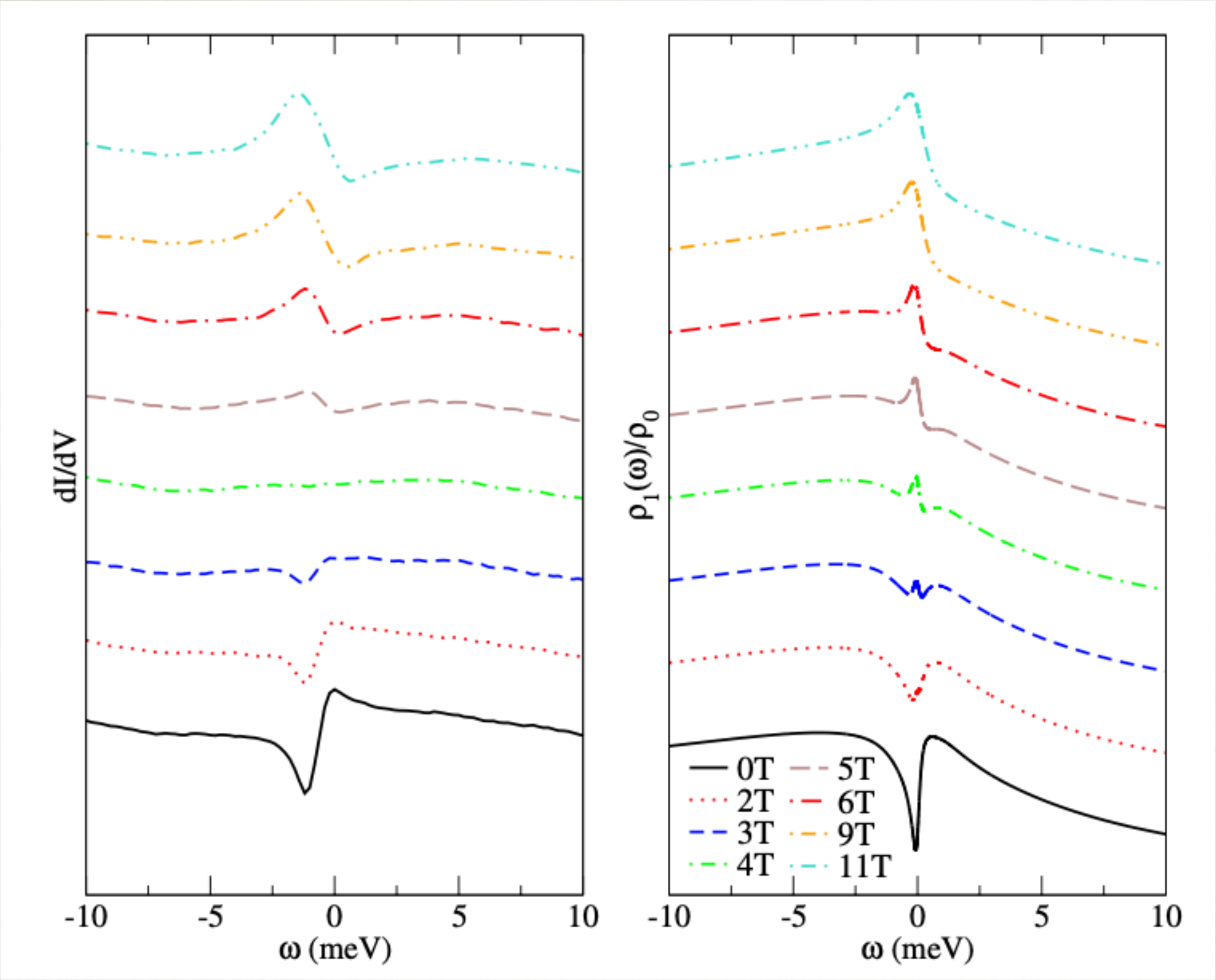


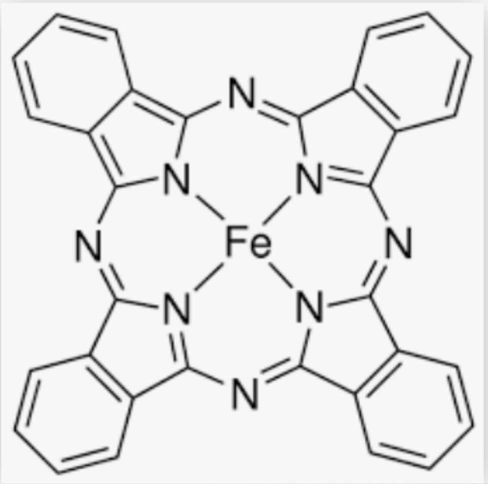


$$\alpha(D,B) \sim -\frac{1}{2}\mathrm{Im}\ln|D_c - D - iB|$$

R. Žitko, G. Blesio, N. Luiz, A. Aligia, Nat. Commun. (2021)

Iron phthalocyanine (FePC) molecules on Au(111) surface





Experimental data:

K. Yang, H. Chen, Th. Pope, Y. Hu, L. Liu, D. Wang, L. Tao, W. Xiao, X. Fei, Y-Y. Zhang, H-G Luo, S. Du, T. Xiang, W. A. Hofer, and H-J. Gao, Nature Commun. 10, 1038 (2019).