Kondo effect in metals and nanostructures

Ramón Aguado ICMM-CSIC

Bibliography:

- A. C. Hewson "The Kondo problem to heavy fermions", Cambridge University Press, 1997.

- P. Coleman, "Introduction to Many Body Physics" (chapters 16 and 17), Cambridge University Press , 2015

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Outline

- Historical introduction: first experimental puzzles.

- Theoretical developments that led to the understanding of the Kondo effect in metals:

    - the Anderson and Kondo models.
    - Kondo's calculation.
    - Anderson's poor's man scaling.
    - Non-perturbative approaches.
    - Strong coupling: the Kondo resonance.

- The two-impurity Kondo problem, generalization to the lattice (slave bosons and 1/N expansions) and relevance to heavy fermion materials.

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Lecture I

- The two-impurity Kondo problem, generalization to the lattice (slave bosons and 1/N expansions) and relevance to heavy fermion materials.

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Lecture II

- The two-impurity Kondo problem, generalization to the lattice (slave bosons and 1/N expansions) and relevance to heavy fermion materials.

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Outline

- Modern aspects of the Kondo effect in mesoscopic systems: quantum dots and nanotubes, non-equilibrium effects, etc.

- New developments: hybrid systems (competition between superconductivity and Kondo), Shiba states, etc.

Lecture III

The Anderson Model

Scattering resonance

"Atomic" limit

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{\sigma} \varepsilon_d n_{d\sigma}$$

$$+ \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

- Paradigm model of strong correlations
- Despite its apparent simplicity, extremely nontrivial: strong on-site interactions+quantum fluctuations

Anderson, Phys. Rev. 124, 41, 1961

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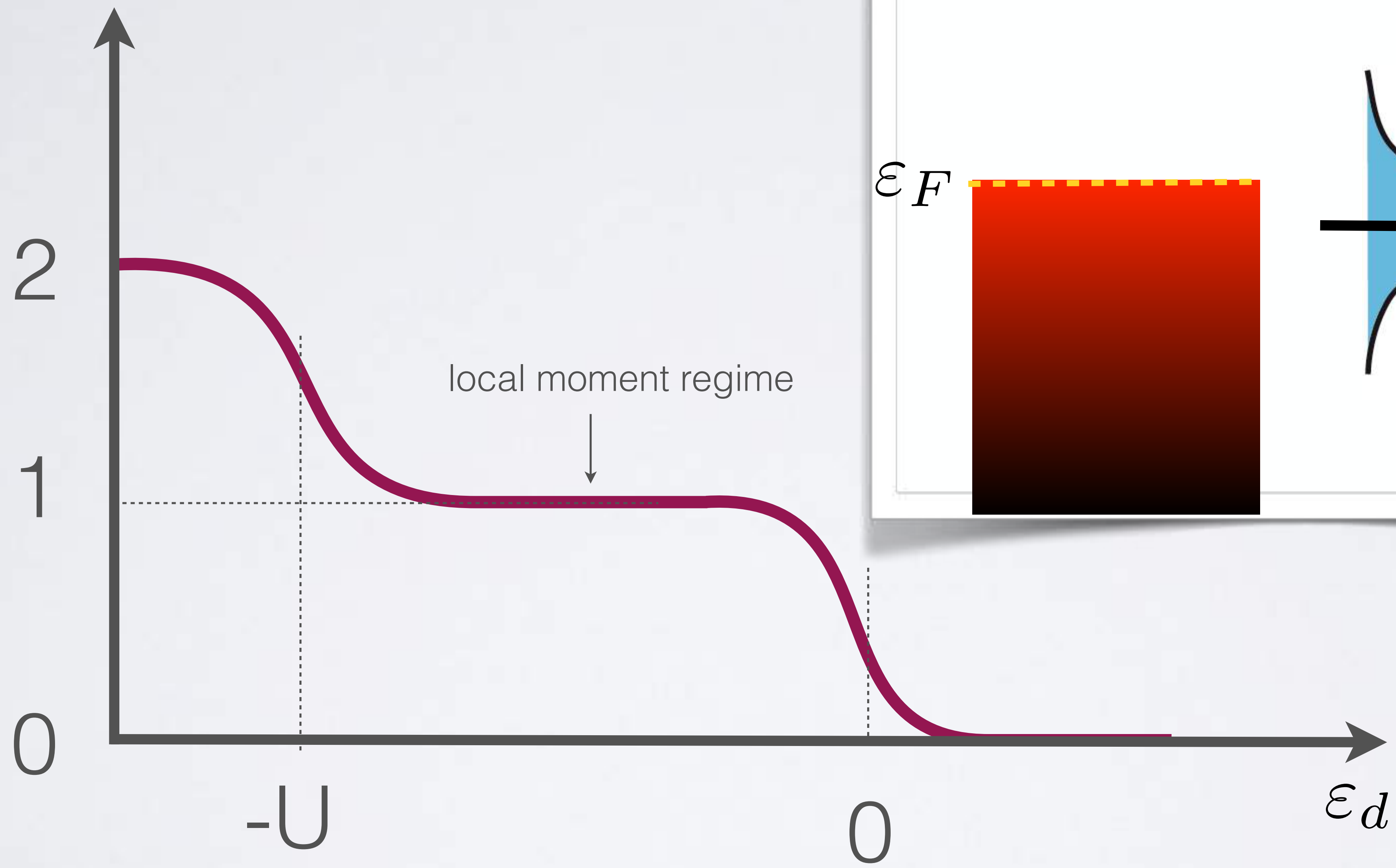
Physics of the Anderson model

$$n_d \equiv \langle n_{d\uparrow} + n_{d\downarrow} \rangle$$



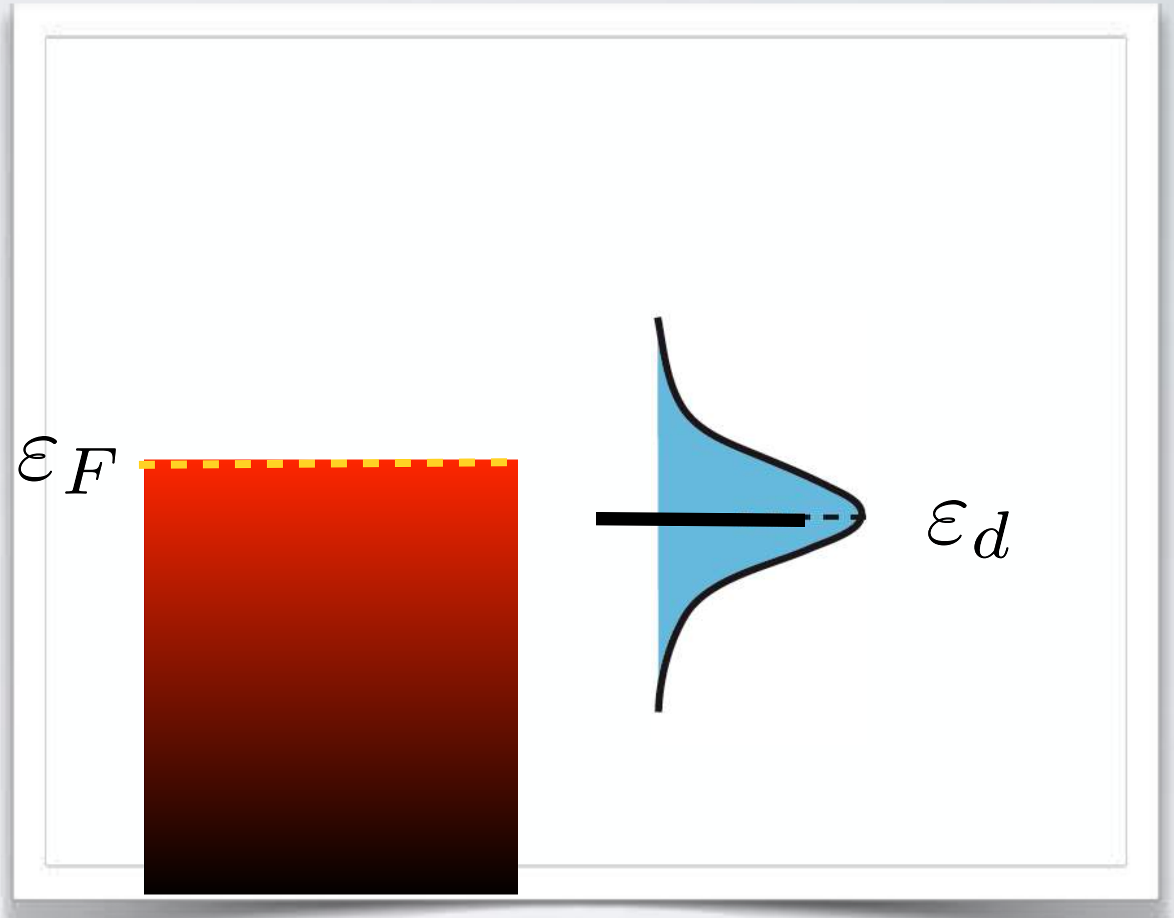
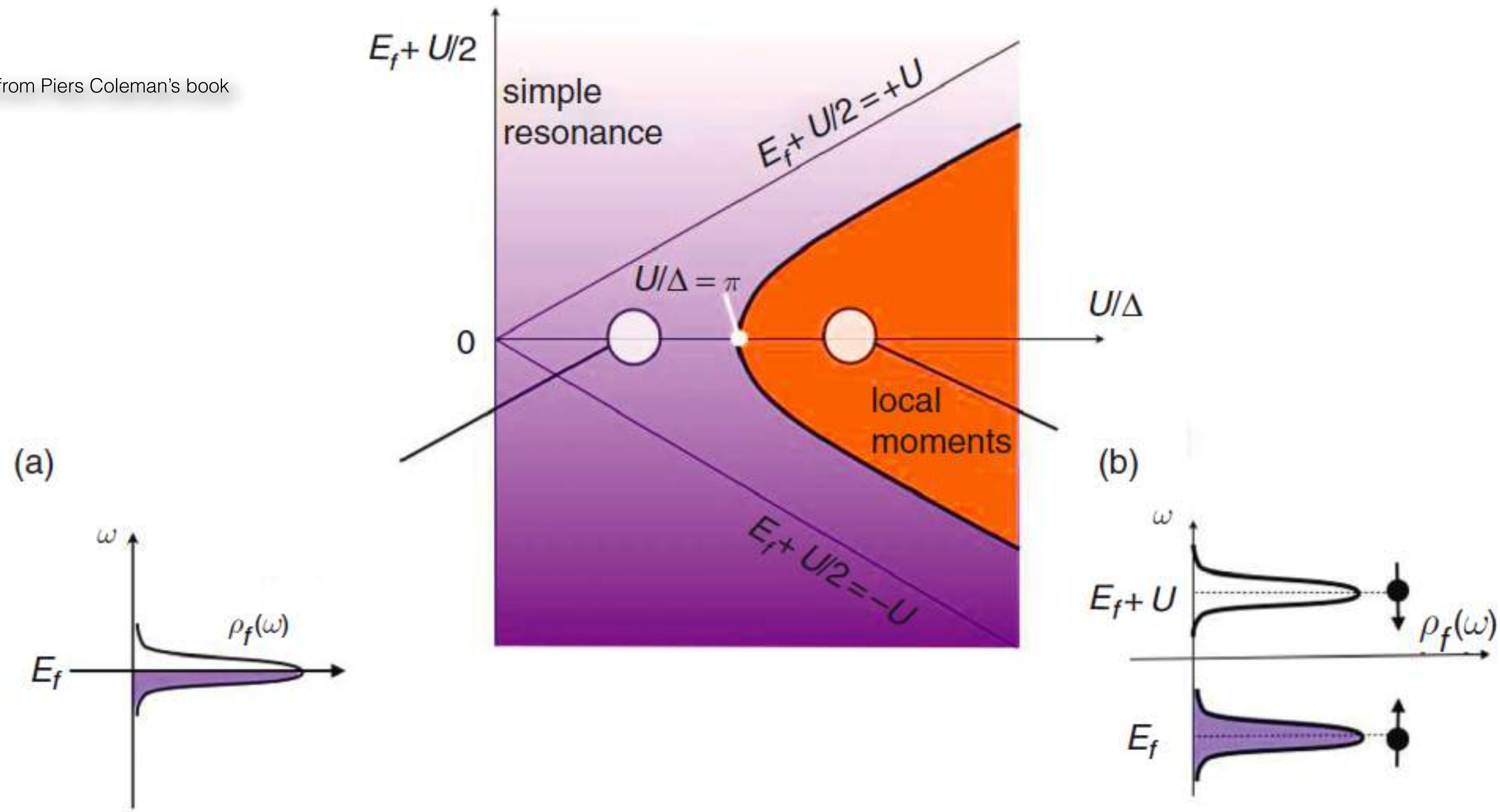


Image from Piers Coleman's book



Quenching of local moments: Kondo's calculation

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{\sigma} \varepsilon_d n_{d\sigma} + \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

$$\Rightarrow \quad H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + J\vec{S}.\vec{s}$$

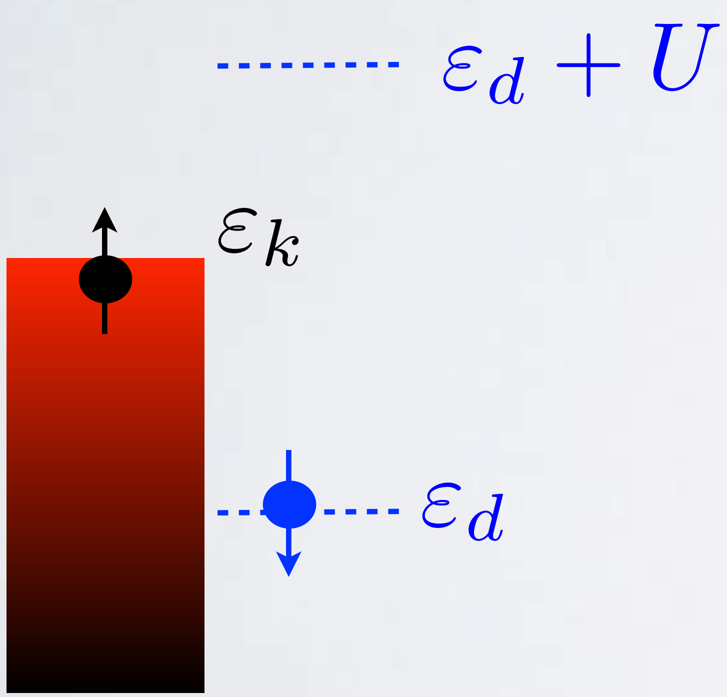
The basic idea is the following: second-order virtual processes in the Anderson model that lead to scattering of a conduction electron with a local moment. Such processes have amplitudes

$$V_{kd} \frac{1}{E_i - E_{int}} V^*_{k'd}$$

initial (E_i) intermediate (E_{int})

Quenching of local moments: Kondo's calculation

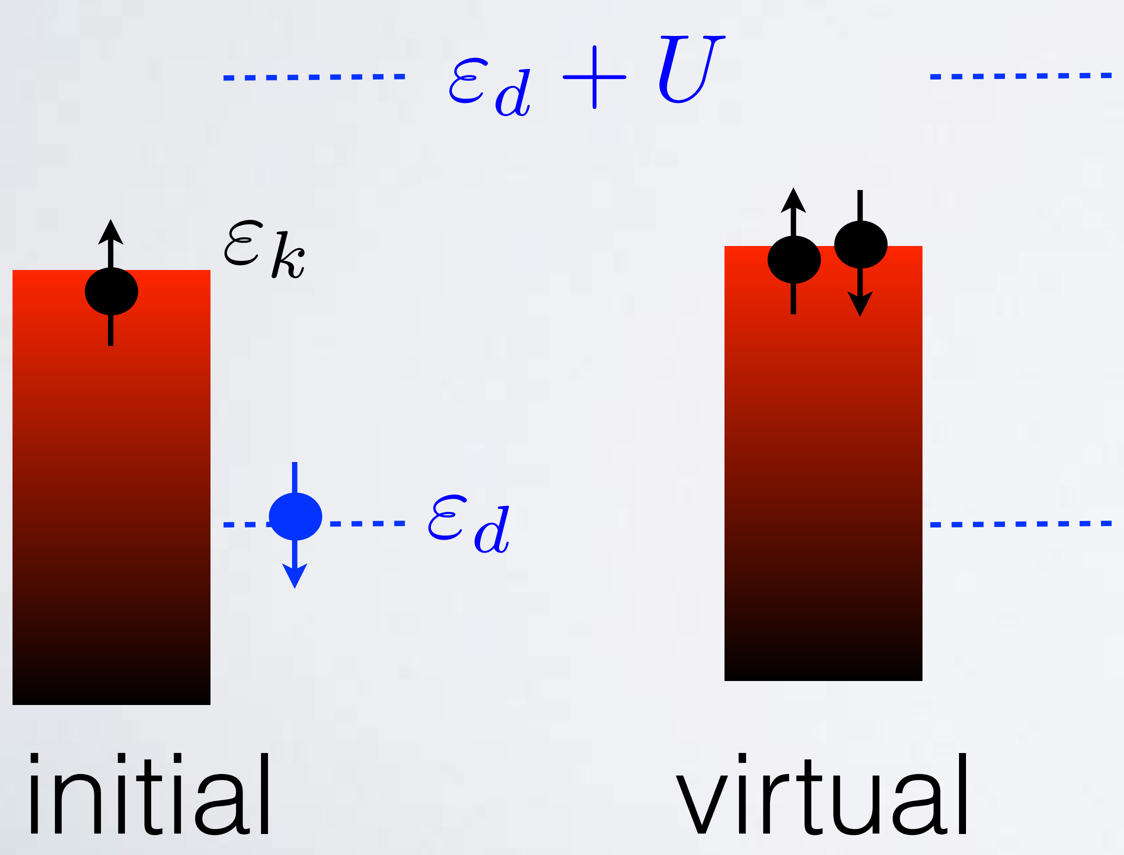
$$V_{kd}\frac{1}{E_i - E_{int}}V^*_{k'd}$$



initial

Quenching of local moments: Kondo's calculation

$$V_{kd}\frac{1}{E_i - E_{int}}V^*_{k'd}$$

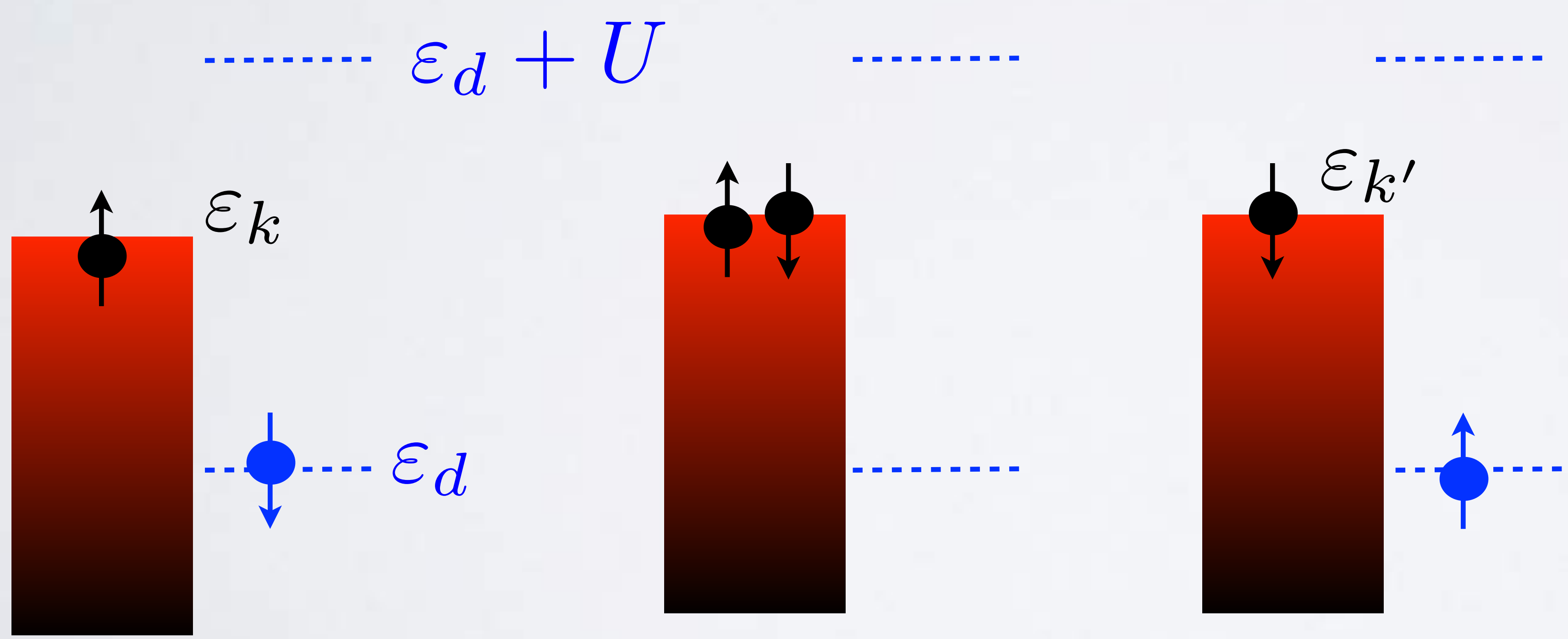


Quenching of local moments: Kondo's calculation

$$T_{k\uparrow,d\downarrow\to k'\downarrow,d\uparrow} \sim -V_{kd}\frac{1}{\varepsilon_d}V^*_{k'd}$$

we have exchanged two fermions

$$\varepsilon_k \approx \varepsilon_{k'} \approx 0$$

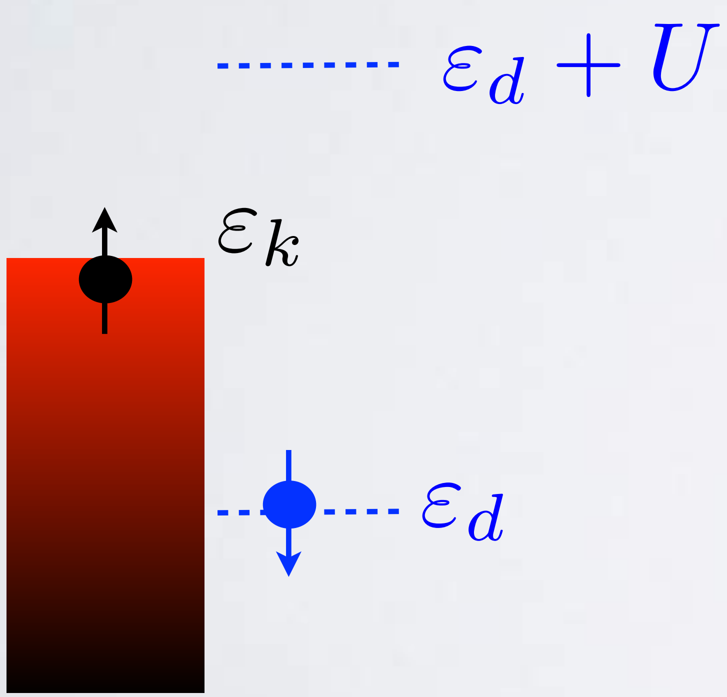


initial virtual final

Spin-flip.

Quenching of local moments: Kondo's calculation

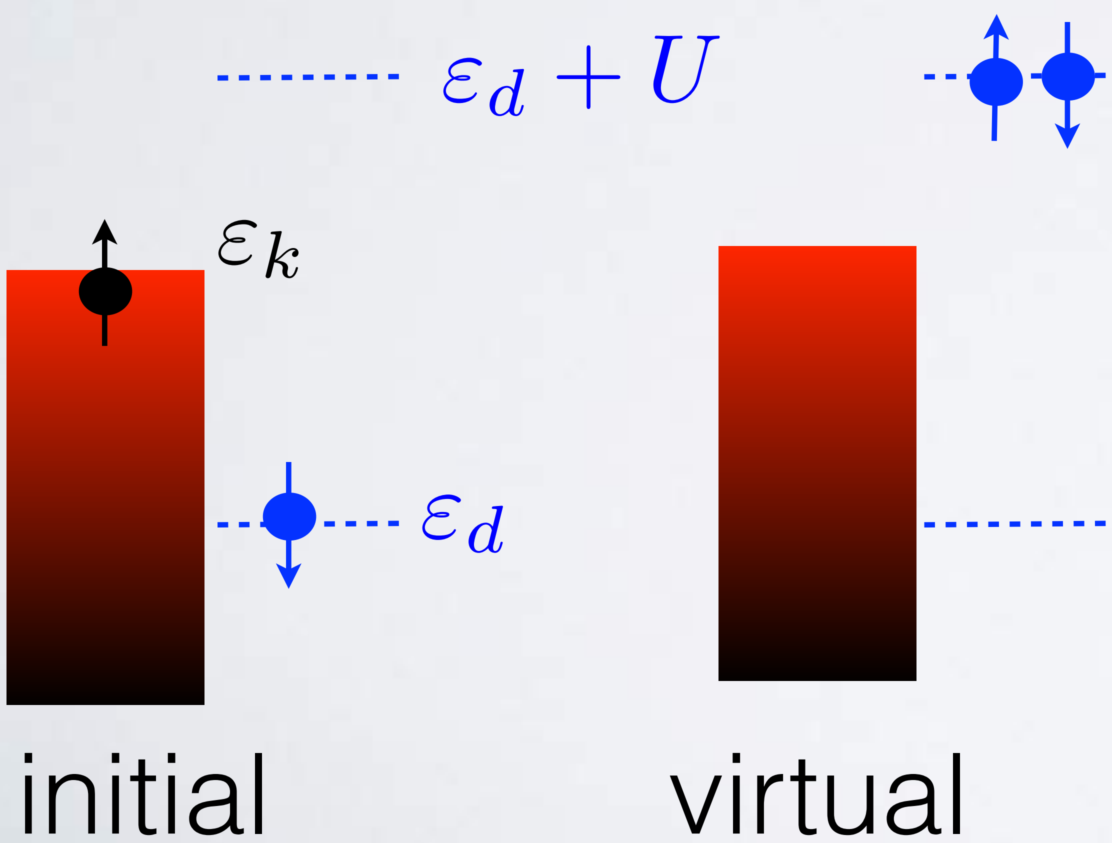
$$V_{kd}\frac{1}{E_i - E_{int}}V^*_{k'd}$$



initial

Quenching of local moments: Kondo's calculation

$$V_{kd}\frac{1}{E_i - E_{int}}V^*_{k'd}$$

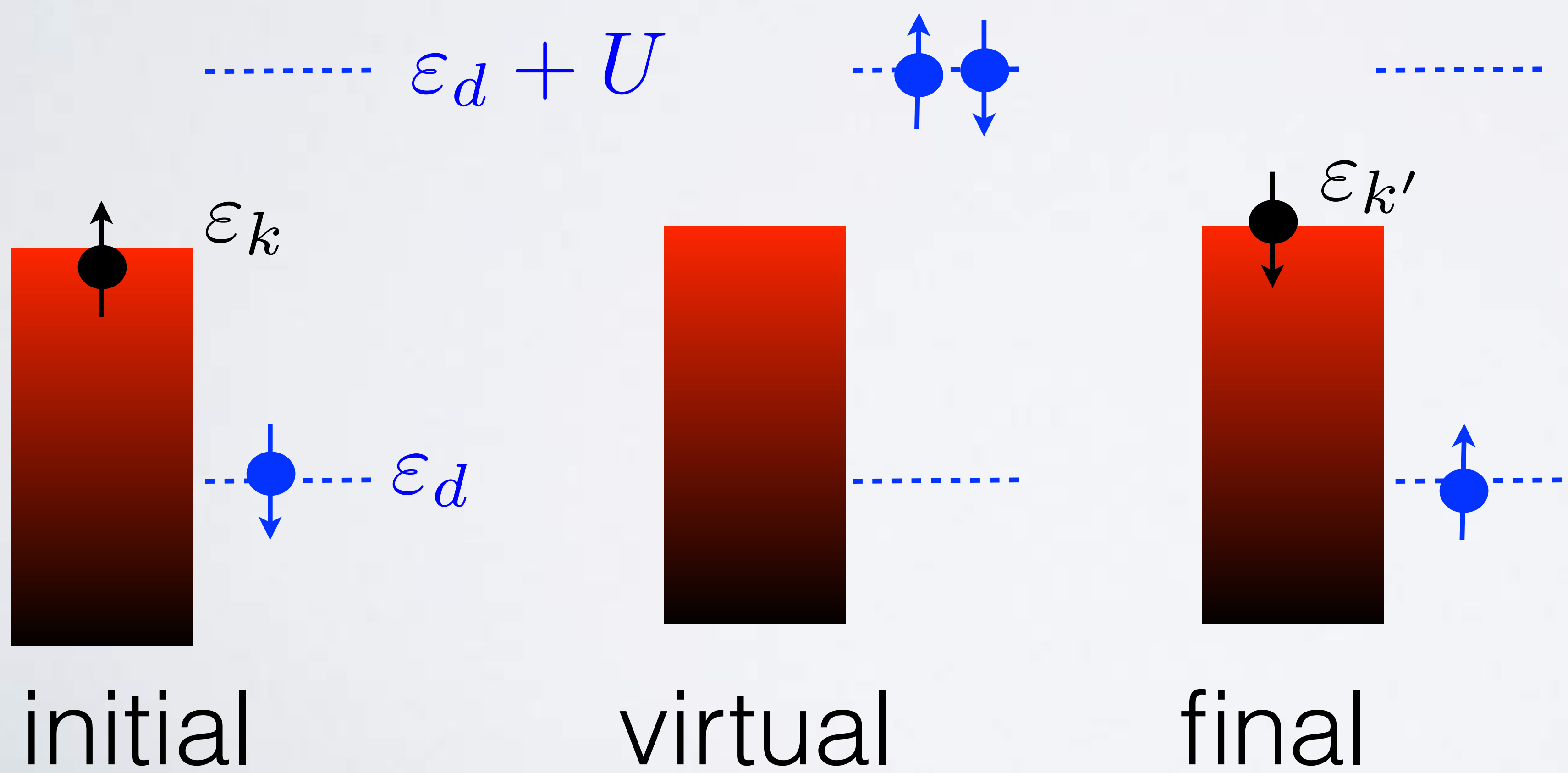


Quenching of local moments: Kondo's calculation

$$T_{k\uparrow,d\downarrow\rightarrow k'\downarrow,d\uparrow} \sim -V_{kd}\frac{1}{-\varepsilon_d - U}V^*_{k'd}$$

we have exchanged two fermions

$$\varepsilon_k \approx \varepsilon_{k'} \approx 0$$



Spin-flip.

$$J_{kk'} = 2V_{kd}V^*_{k'd}\left(\frac{1}{\varepsilon_k - \varepsilon_d - U} + \frac{1}{\varepsilon_d - \varepsilon_{k'}}\right)$$

$\varepsilon_k \approx \varepsilon_{k'} \approx 0$

$$J_{eff} = 2|V_{kd}|^2\left(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_d + U}\right) = \frac{2\Gamma}{\pi}\left(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_d + U}\right)$$

Kondo showed that a logarithmic correction appears in a perturbative expansion in terms of J (Prog. Theor. Phys. **32**, 37, 1964).

$$H_K = \sum_{k,\sigma} \varepsilon_k n_{k,\sigma} - \sum_{k,k'} \frac{J_{kk'}}{\hbar^2}(\Psi^\dagger_{k'} S \Psi_k).(\Psi^\dagger_d S \Psi_d)$$

Quenching of local moments: Kondo's calculation

$$R = \frac{3\pi c_{imp} m J^2}{2e^2\hbar\varepsilon_F} S(S+1)(1 - 4J\rho(0) ln\frac{k_B T}{D}) + O(J^4)$$

$$R(T) = AT^5 - Bln\frac{k_B T}{D}$$

If we add the phonon term, Kondo's calculation explains the resistance minimum.

Progress of Theoretical Physics, Vol. 32, No. 1, July 1964

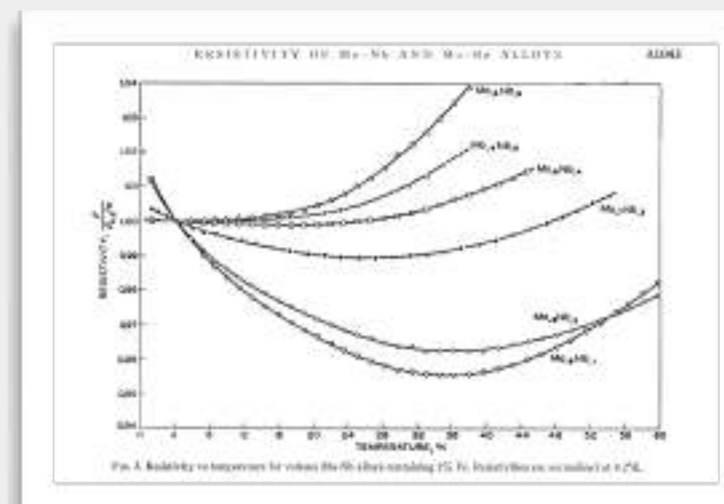
Resistance Minimum in Dilute Magnetic Alloys

Jun KONDO

Electro-technical Laboratory
Nagatacho, Chiyodaku, Tokyo

(Received March 19, 1964)

Based on the *s-d* interaction model for dilute magnetic alloys we have calculated the scattering probability of the conduction electrons to the second Born approximation. Because of the dynamical character of the localized spin system, the Pauli principle should be taken into account in the intermediate states of the second order terms. Thus the effect of the Fermi sphere is involved in the scattering probability and gives rise to a singular term in the resistivity which involves $c \log T$ as a factor, where c is the concentration of impurity atoms. When combined with the lattice resistivity, this gives rise to a resistance minimum, provided the *s-d* exchange integral J is negative. The temperature at which the minimum occurs is proportional to $c^{1/5}$



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Quenching of local moments: Kondo's calculation

$$R = \frac{3\pi m J^2}{2e^2\hbar\varepsilon_F} S(S+1)(1 - 4J\rho(0) ln\frac{k_B T}{D})$$

- More relevant: the resistivity diverges as $T \to 0$

The solution of this Non-perturbative problem is what is known as the **Kondo problem**. More than three decades of theory work towards solving this problem helped to develop a great deal of strongly correlated electron techniques.

- Scaling: Anderson 60's
- Numerical renormalization group: Wilson 70's, Nobel prize.
- Fermi liquid: Langreth, Nozieres, 70's
- Exact solutions by Bethe Anstaz: Andrei, Wiegman, 80's
- 1/N expansions 80's, 90's
- Non-equilibrium properties, 2000-present

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Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$g(D') = \frac{1}{2}\frac{1}{ln[\frac{D'}{T_K}]}$$

"Running" coupling constant

The effective coupling diverges at a dynamically generated scale: the **Kondo temperature**.

$$T_K = D_0 exp[-1/2g_0]$$

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Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$\frac{\partial ln g}{\partial ln(D_0/D)} = 2g + O(g^2)$$

↓

$$g(D') = \frac{g_0}{1 - 2g_0 ln(D_0/D')}$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

Ferromagnetic case

$$g(D') = -\frac{|g_0|}{1 + 2|g_0| ln(D_0/D')}$$

Very gradual decreasing of the effective coupling of the local moment to the surrounding conduction sea. Irrelevant since the interaction scales to zero (the problem remains perturbative).

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

Antiferromagnetic case

$$g(D') = \frac{g_0}{1 - 2g_0 ln(D_0/D')} = \frac{1}{2} \frac{1}{ln[\frac{D'}{D_0 exp(-1/2g_0)}]}$$

$$2g(D') = \frac{1}{ln(D'/T_K)}$$

$$T_K = D_0 exp[-1/2g_0]$$

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Breakthrough: Anderson's scaling ideas

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Antiferromagnetic case

$$2g(D') = \frac{1}{ln(D'/T_K)}$$

The effective coupling diverges at a **dynamically generated scale**: the Kondo temperature.

$$T_K = D_0 exp[-1/2g_0]$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

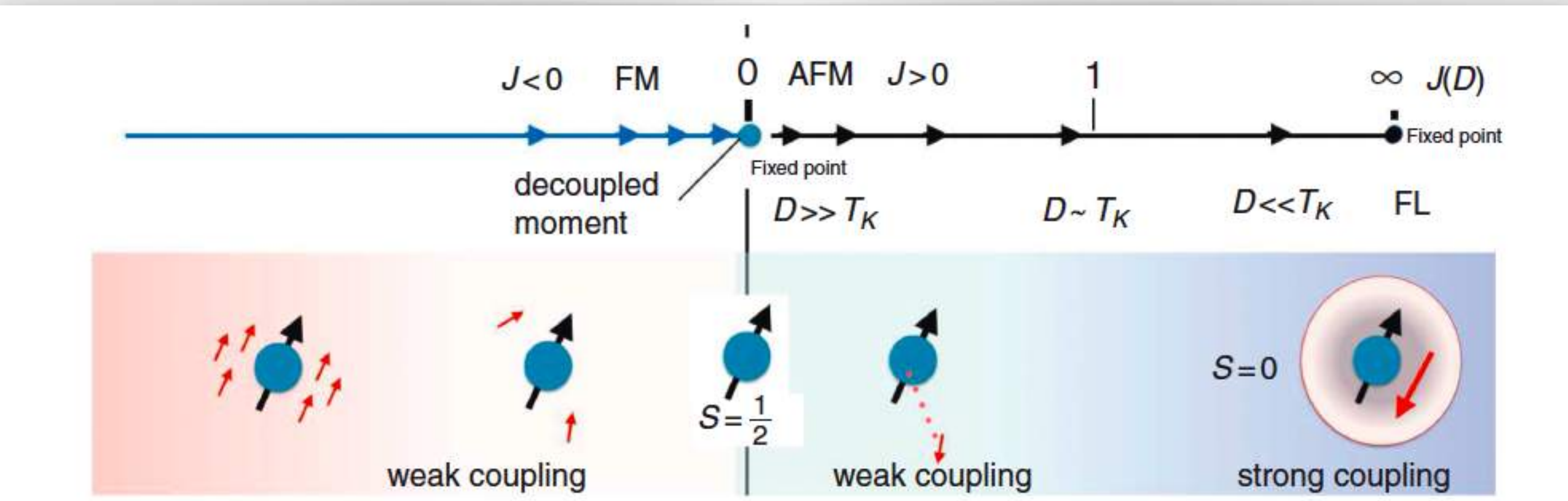
- The Kondo interaction can only be treated perturbatively at energies larger compared with the Kondo temperature.
- The Kondo problem does not depend on the high-energy details of the model but rather on one relevant energy scale, the Kondo temperature

$$T_K = D_0 exp[-1/2g_0]$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$T_K = D_0 exp[-1/2g_0]$$



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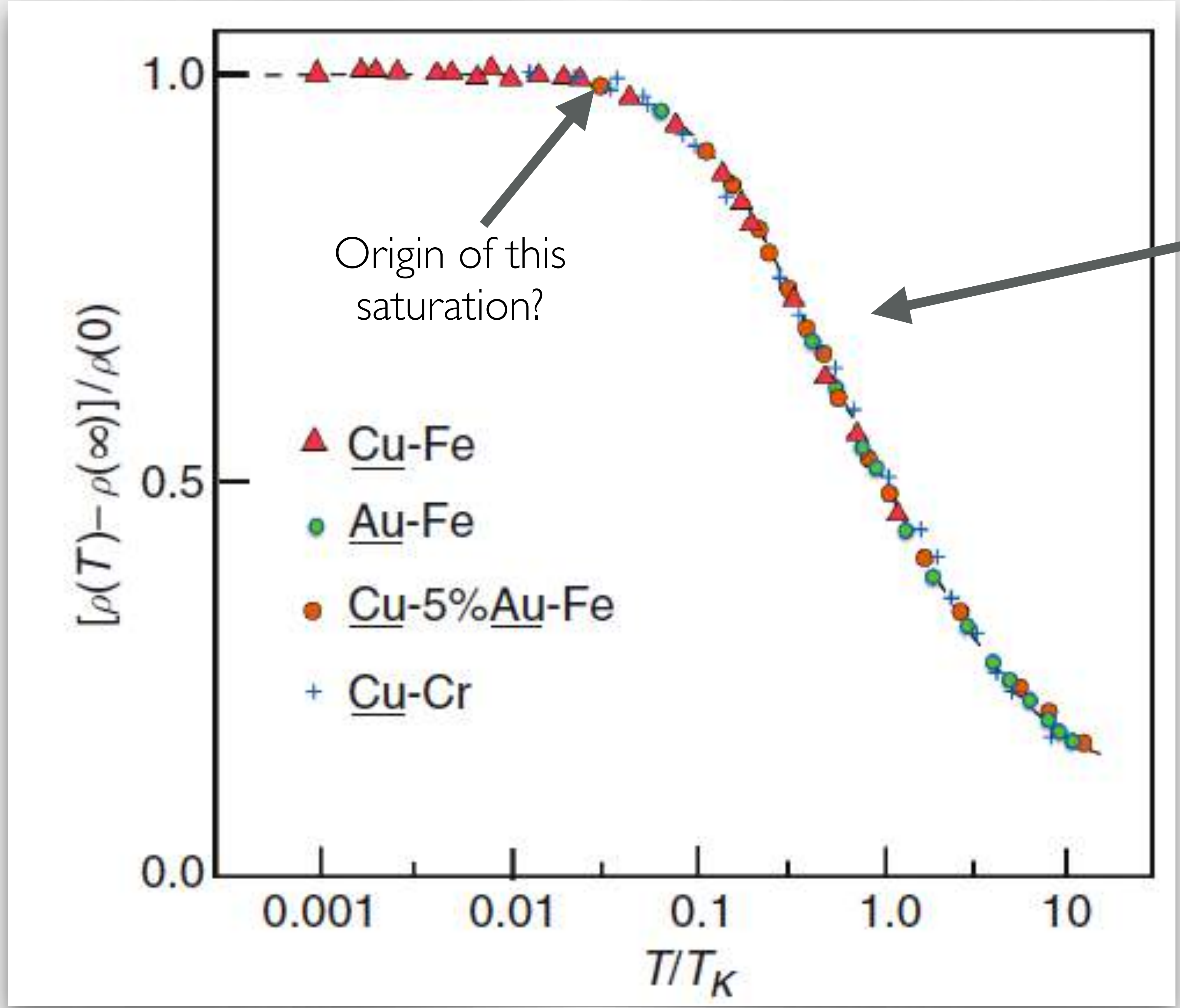
Anderson's scaling ideas

All logarithmic corrections vanish when the high-energy cutoff equals the thermal energy:

$$g(k_B T) = \frac{1}{2}\frac{1}{ln[\frac{T}{T_K}]}$$

- The Kondo temperature is the only scale governing the physics.
- Different systems have the same low-temperature behavior.
- <u>All</u> physical quantities depend on temperature only through this logarithm (universal behavior).



Universality: all curves fall on top of each other, details don't matter!!

•The first reliable non-perturbative calculation to go well below the Kondo temperature was Wilson's numerical renormalization group (Review of Modern Physics 47, 773, 1975).

•The renormalization group approach was designed for problems in which there is no characteristic energy or length scale and every energy or length makes a contribution such as critical phenomena and phase transitions. This is also the case with the Kondo problem as the integrals that lead to breakdown of perturbation theory are logarithmic.

$$\int_{k_B T}^{D} \frac{d\varepsilon}{\varepsilon} \sim ln(\frac{k_B T}{D})$$

• we cannot take the $D \to \infty$ limit: high energy states matter.

Ultraviolet divergence

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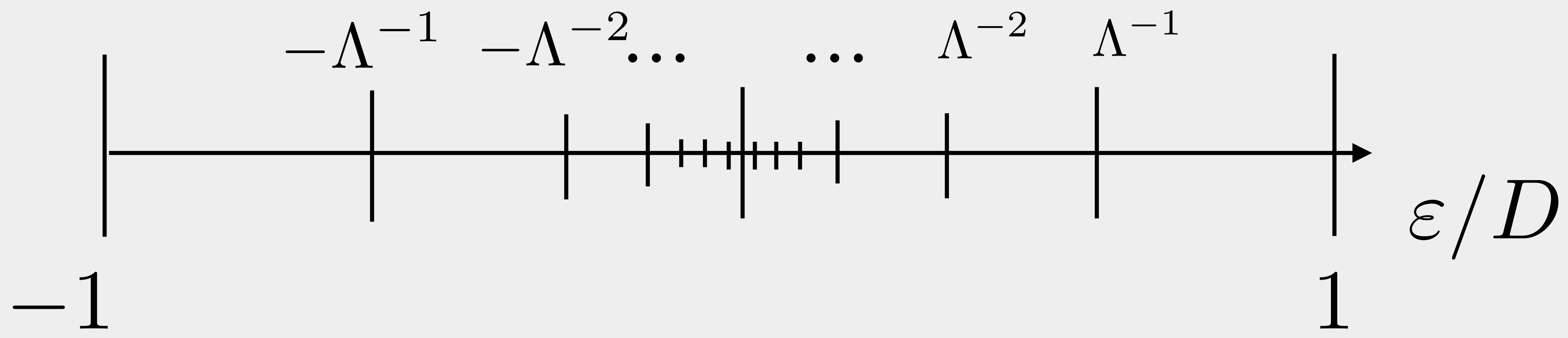
- To reflect this dependence, Wilson designed a logarithmic discretization of the states of the conduction band.



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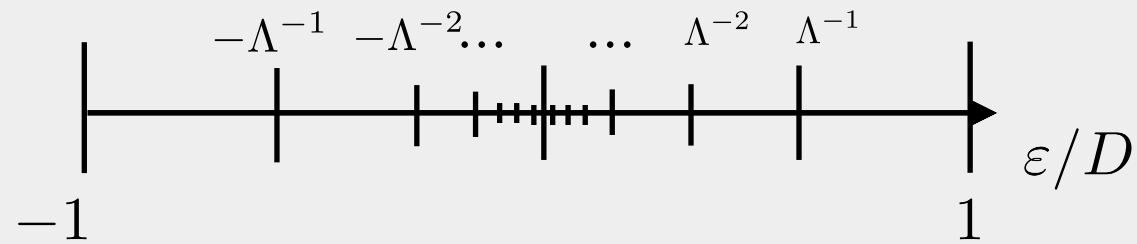
- Tight-binding chain



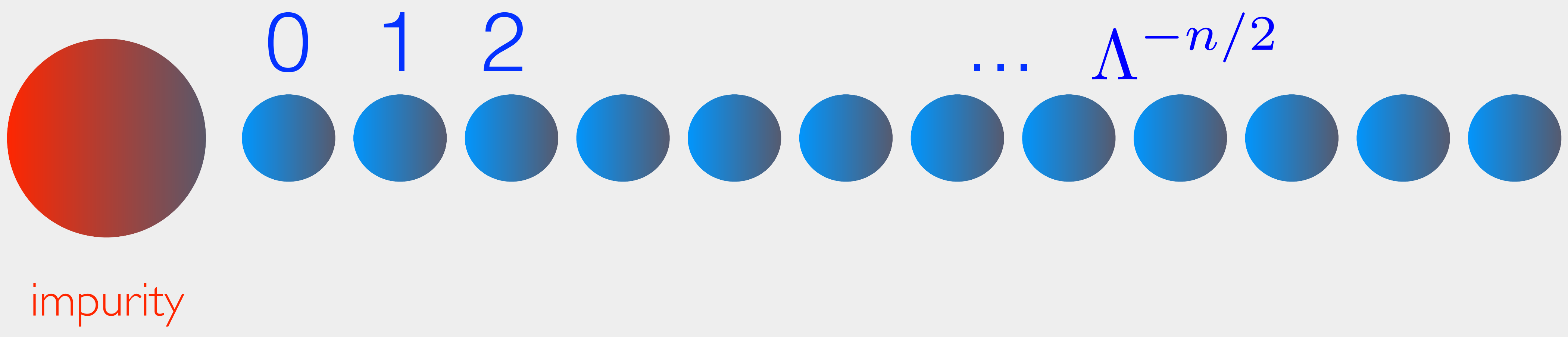
$$H = J\rho \sum_{\sigma,\sigma'} S.c^{\dagger}_{0,\sigma} s_{\sigma,\sigma'} c_{0,\sigma} + \sum_{n=0}^{\infty} \sum_{\sigma} (t_n c^{\dagger}_{n,\sigma} c_{n+1,\sigma} + t_n^* c^{\dagger}_{n+1,\sigma} c_{n,\sigma})$$

$$t_n \approx \frac{1+\Lambda^{-1}}{2\Lambda^{n/2}}$$

- The first reliable non-perturbative calculation to go well below the Kondo temperature was Wilson's numerical renormalization group (Review of Modern Physics 47, 773, 1975).

- The low-energy part of the spectrum is obtained by iterative diagonalization adding one extra site of the chain in each step of the iterative scheme.

- The number of states would increase exponentially as new sites are added. This problem is avoided and a numerically tractable scheme is obtained if the higher lying levels are truncated in each step by keeping a fixed number of low-lying levels (typically of order 10^3).

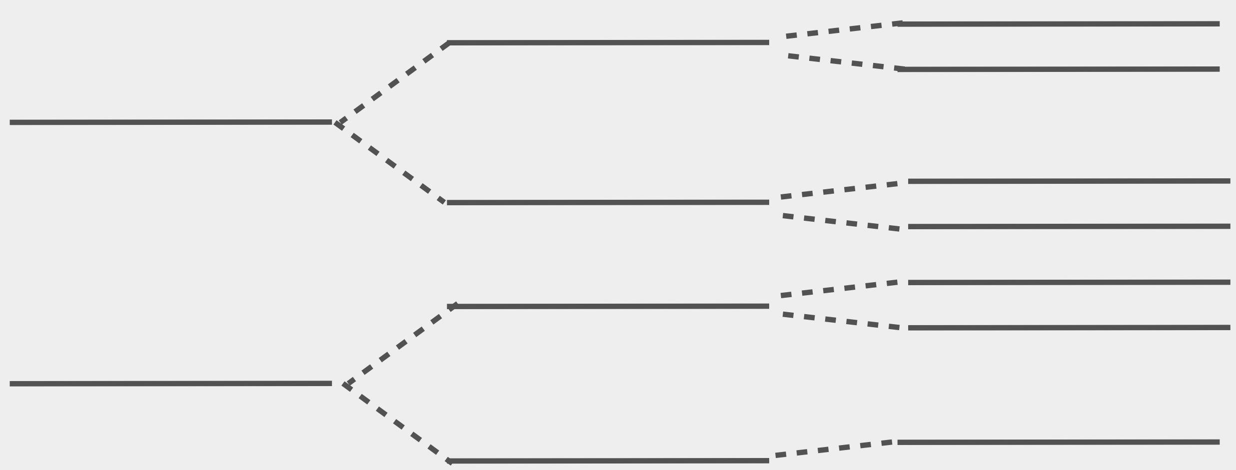


- The first reliable non-perturbative calculation to go well below the Kondo temperature was Wilson's numerical renormalization group (Review of Modern Physics 47, 773, 1975).

- recurrence relation

$$\bar{H}_{N+1} = \Lambda^{1/2}\bar{H}_N + \sum_\sigma (c^\dagger_{N\sigma}c_{N+1\sigma} + c^\dagger_{N+1\sigma}c_{N\sigma})$$

- Many energy scales are locally coupled



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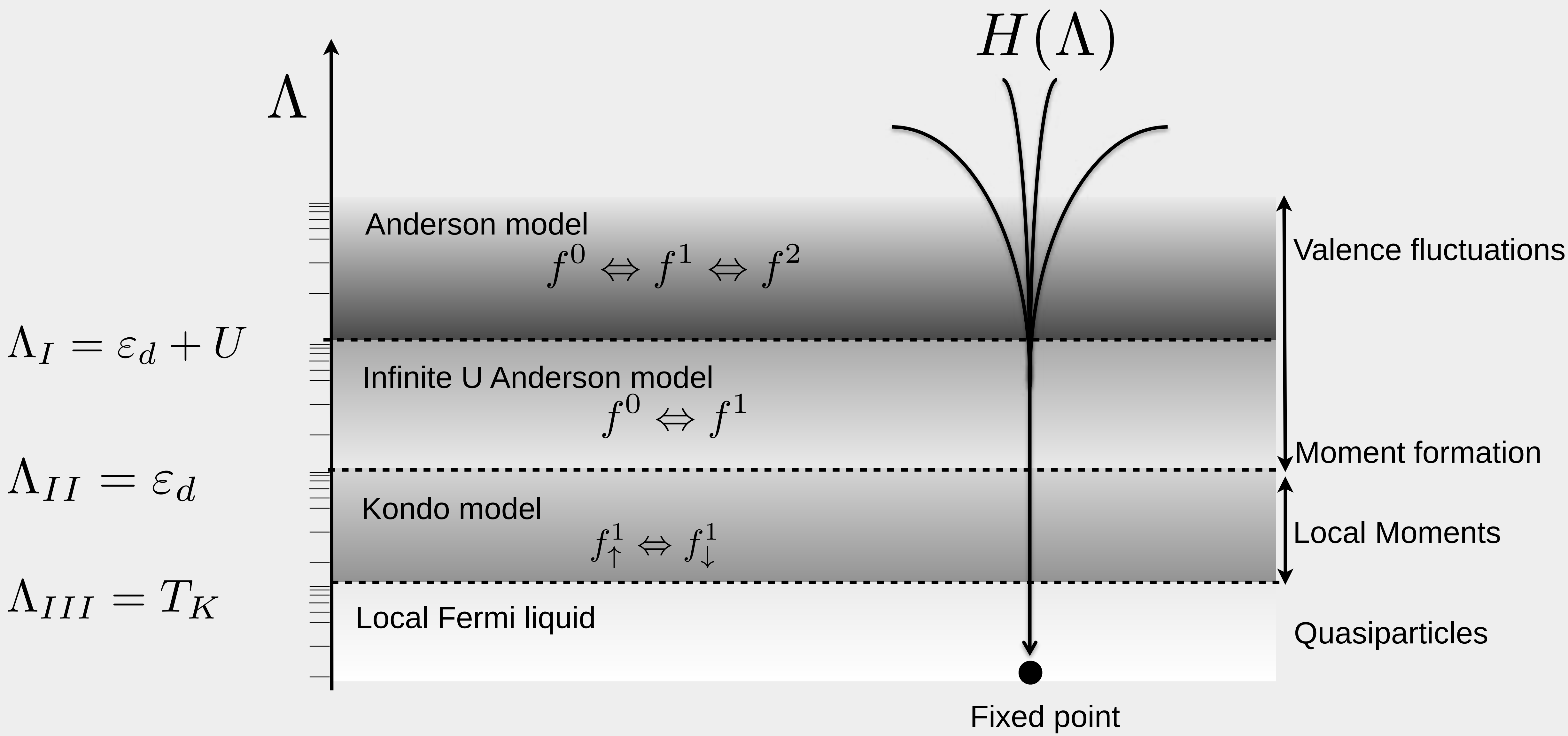
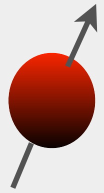


adapted from Piers Coleman, arxiv:0612006

Asymptotic freedom in condensed matter

The Kondo effect is a manifestation of the phenomenon of "asymptotic freedom" that also governs quark physics. Like the quark, at high energies the local moments inside metals are asymptotically free, but at energies below a characteristic scale, the Kondo temperature, they interact so strongly with the surrounding electrons that they become screened into a singlet state, or "confined" at low energies, ultimately forming a Landau Fermi liquid.

$$J(\Lambda) = 0$$



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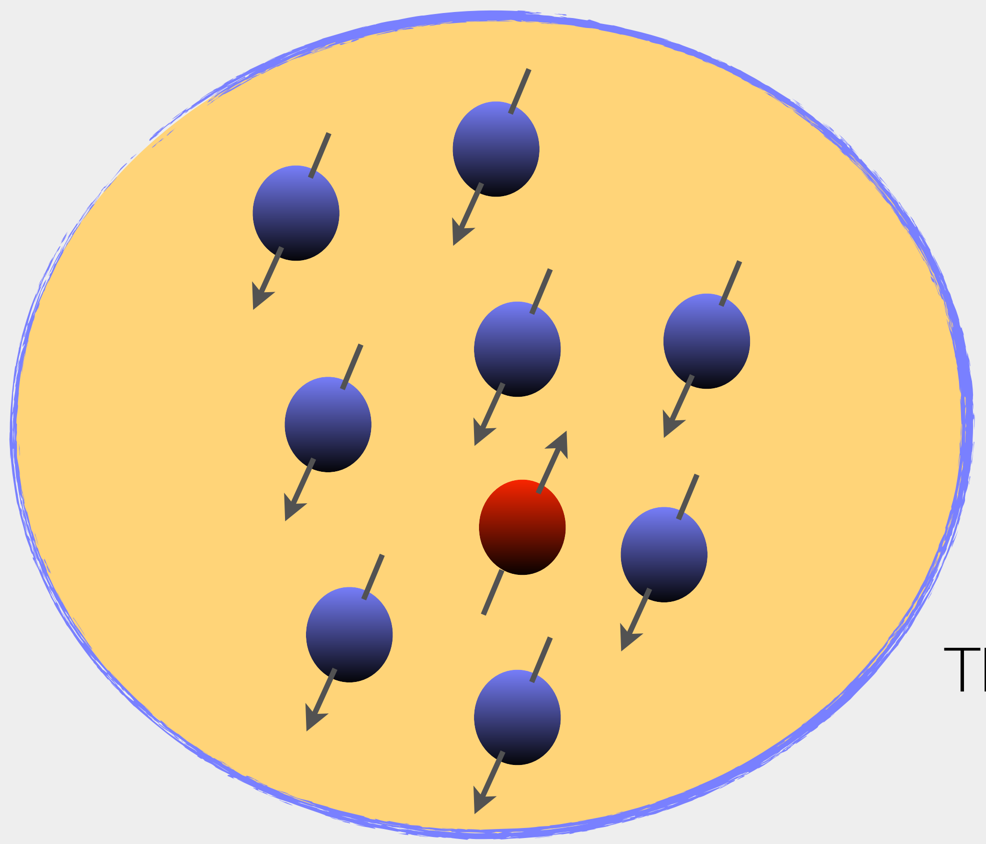
$$J(\Lambda) = 0$$

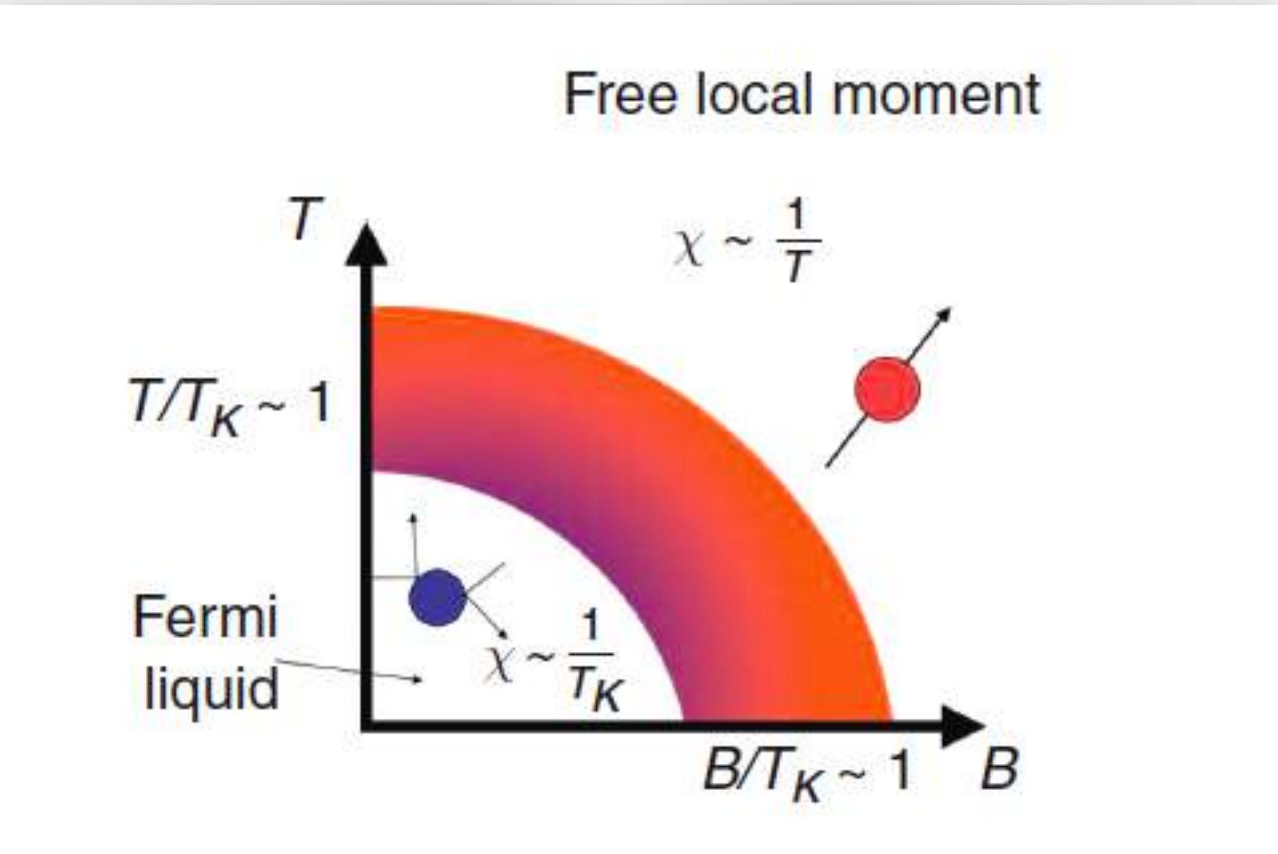
$$J(\Lambda) = \infty$$

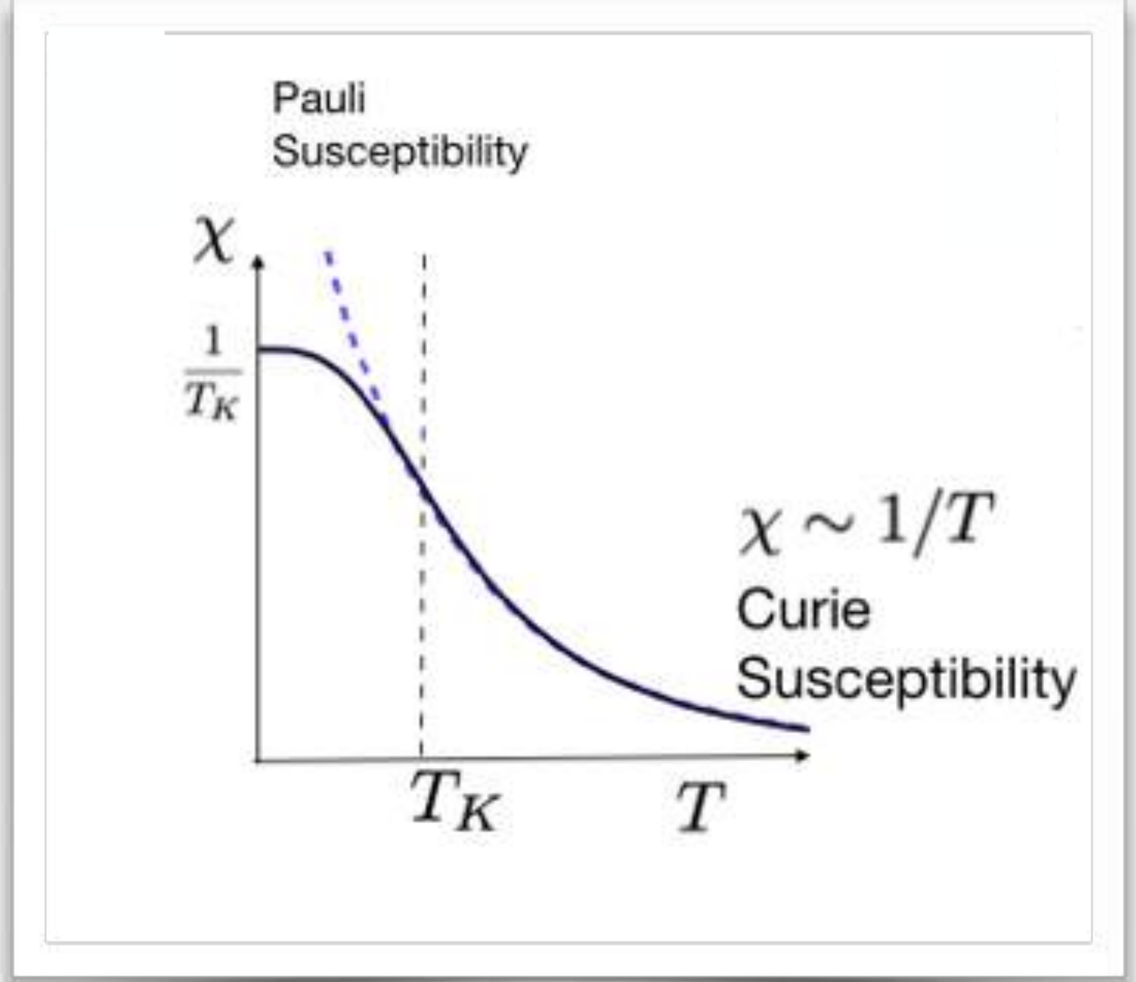


$$\xi_K \simeq \frac{\hbar v_F}{k_B T_K}$$

This "Kondo cloud" is extremely long!!!

Asymptotic freedom in condensed matter

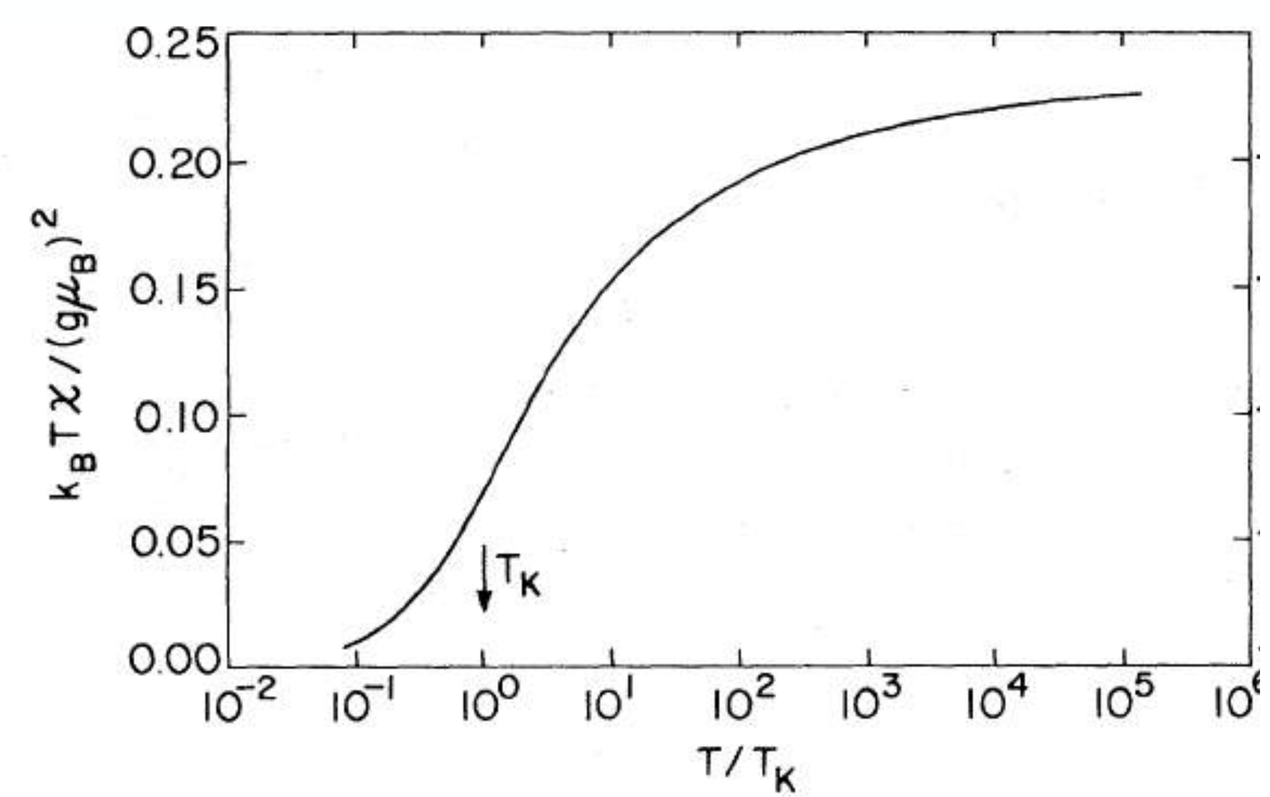




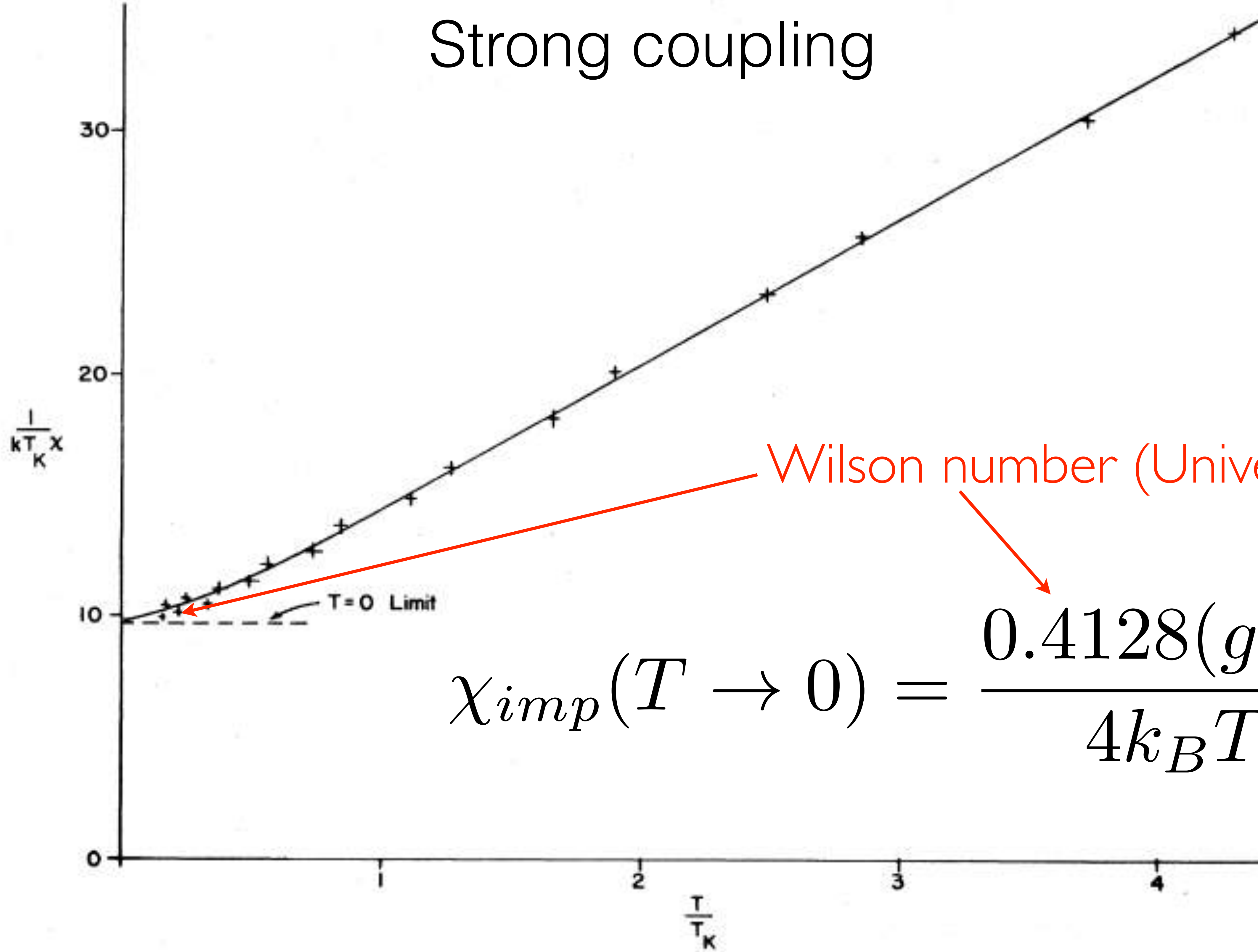
Crossover region

$$\chi_{imp}(T) = \frac{0.68(g\mu_B)^2}{4k_B(T+\sqrt{2}T_K)}$$

Curie-Weiss form that corresponds to a reduced moment with respect to the free spin. Even for temperatures of the order of the Kondo temperature, the impurity moment is around 30% that of a free spin. Very slow approach to the susceptibility of a free spin



Strong coupling



$$\chi_{imp}(T \rightarrow 0) = \frac{0.4128(g\mu_B)^2}{4k_B T_K}$$

FIG. 17. Plot of inverse susceptibility $\chi^{-1}(T)$ vs T from the computer calculations. The magnetic moment and g factor of both the impurity and the conduction band electrons are set equal to 1. The plot actually shows $(kT_K\chi)^{-1}$ vs T/T_K, where T_K was defined in Eq. (IX.94). The crosses represent results for two different calculations (both with $\Lambda = 2.25$, but $\tilde{J} = 0.024$ for one and 0.02412 for the other); the scatter to truncation errors. The zero temperature value is taken from Eq. (IX.69) and Table XVI.

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Fermi liquid fixed point

Wilson was able to show that the specific heat would be a linear function of temperature, like a Fermi liquid, that could be written in a universal form.

$$C_V = \gamma T$$

$$\gamma = \frac{\pi^2}{3}\frac{0.4128 \pm 0.002}{8T_K}$$

$$W = \frac{\chi/\chi^0}{\gamma/\gamma^0} = \frac{\chi}{\gamma}\left(\frac{\pi^2 k_B^2}{3\mu_B^2}\right) = 2$$

The Wilson ratio (the quotient between the susceptibility and the linear specific heat) is also a universal number.

Fermi liquid fixed point

- For low temperatures T, the impurity spin is screened by the spin of conduction electrons.

- The singlet consisting of the impurity spin and the screening cloud scatters other electrons.

- Virtual excitations of the singlet to the triplet state lead to weak interactions between conduction electrons of opposite spin in the vicinity of the impurity.

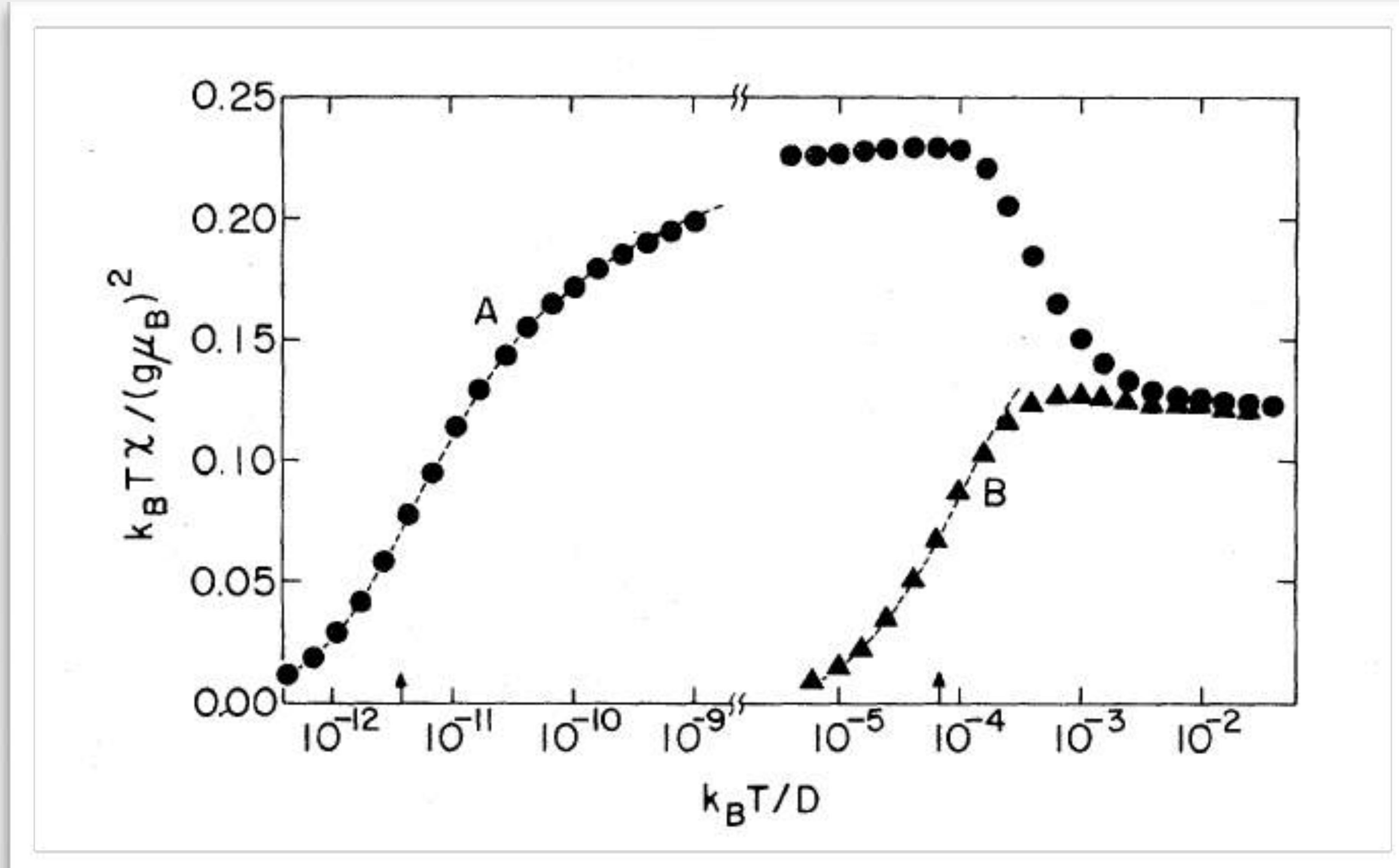
- The length scale for these interactions and for scattering from the impurity spin plus screening cloud is ξ_K which is much larger than the distance between electrons.

- The screening is done by electrons with energy to ε_F

- The impurity not only causes scattering of electrons, it also induces interactions between the electrons. Since these interactions won't change on microscopic length scales, we expect that a description in terms of Fermi Liquid Theory might apply (Nozières 1975).

NRG for the Anderson model

H. R. Krishna-murthy, J. W. Wilkins and K. G. Wilson, Phys. Rev. B 21, 1003–1043; 21, 1044–1083 (1980)



Further confirmation of these ideas came in the form of exact results for the **thermodynamics** of the Kondo model by Andrei (1980) and Wiegmann (1980), by applying the Bethe Ansatz method. Later also for the Anderson model (Wiegmann, 1980).

How about **dynamics**?

How about **dynamics**?

The key quantity is the impurity spectral function

$$\rho_\sigma(\omega) = -\frac{1}{\pi} Im G^r_\sigma(\omega) = -\frac{1}{\pi} Im G_\sigma(\omega + i\eta)$$

$$G_\sigma(\omega) = -i \int_{-\infty}^{\infty} dt \langle T d_\sigma(t) d^\dagger_\sigma(0) \rangle e^{i\omega t}$$

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How about **dynamics**?

Physical meaning

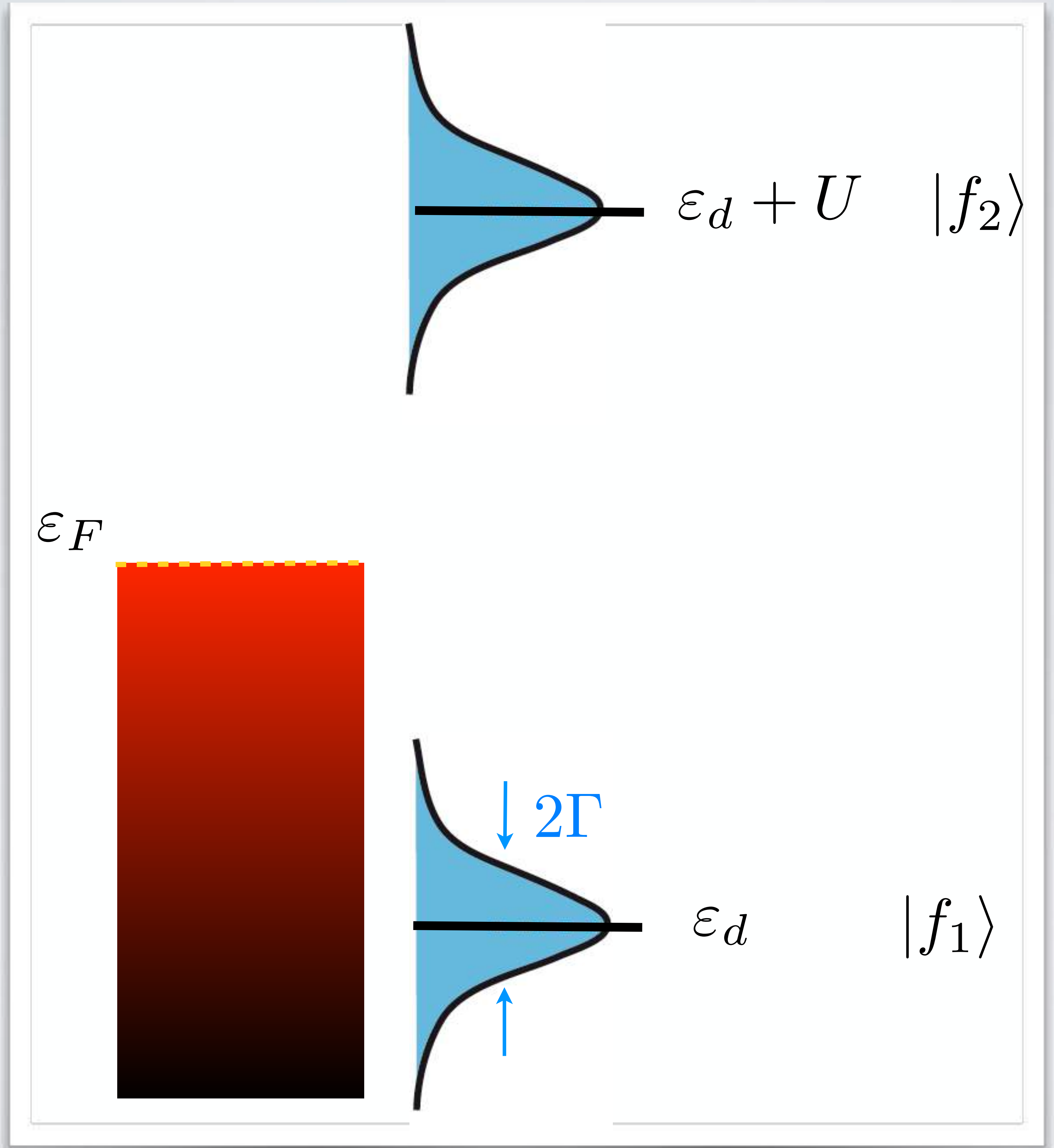
$$\rho_\sigma(\omega) = -\frac{1}{\pi} Im G^r_\sigma(\omega) = -\frac{1}{\pi} Im G_\sigma(\omega + i\eta)$$

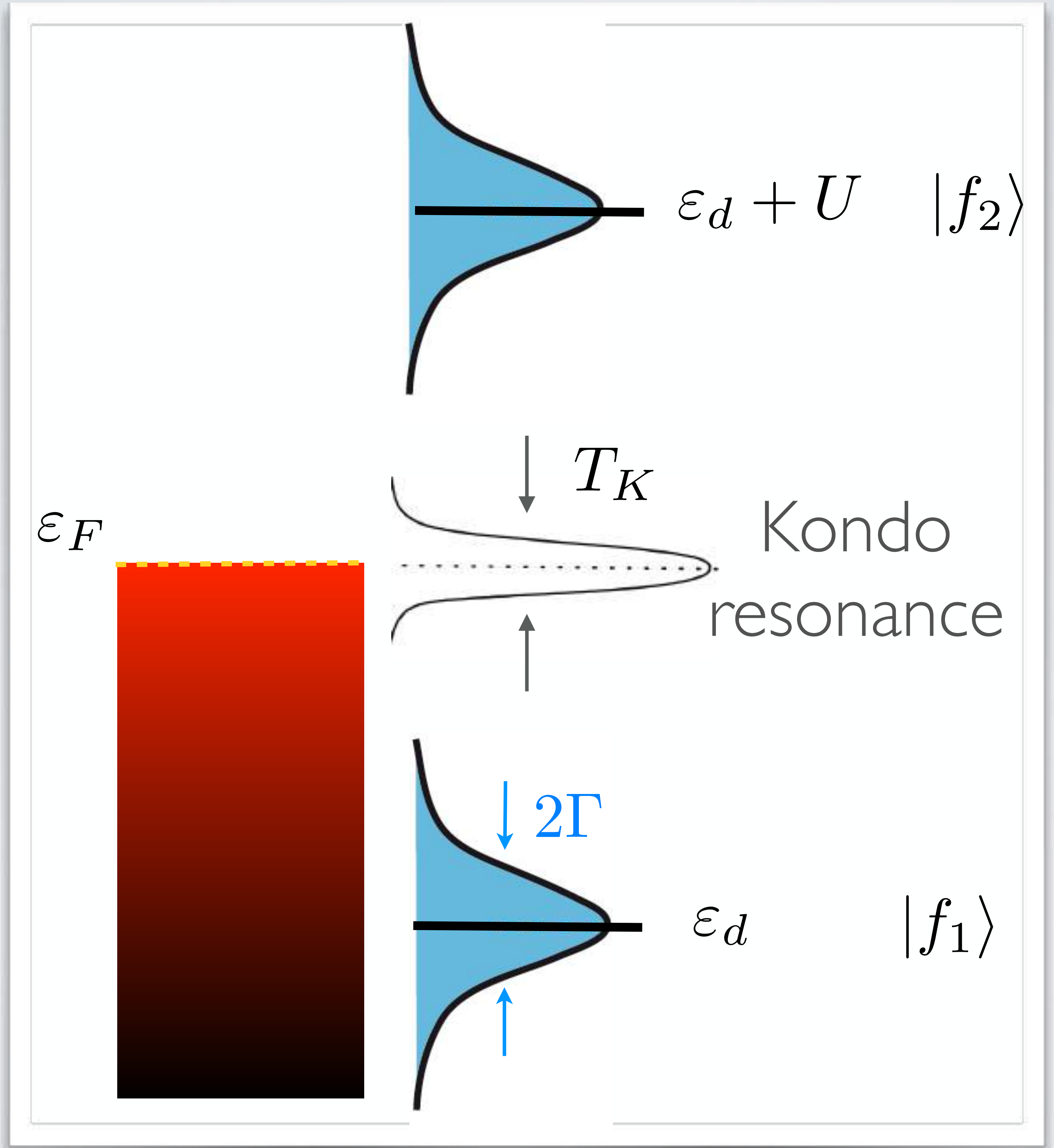
electron addition

$$\rho_\sigma(\omega) = \sum_i |\langle i|d^\dagger_\sigma|0\rangle|^2 \delta(\omega - (E_i - E_0)) \quad \omega > 0$$

electron removal

$$\rho_\sigma(\omega) = \sum_i |\langle i|d_\sigma|0\rangle|^2 \delta(\omega - (E_0 - E_i)) \quad \omega < 0$$


$\varepsilon_d + U$
$|f_2\rangle$
ε_F
2Γ
ε_d
$|f_1\rangle$



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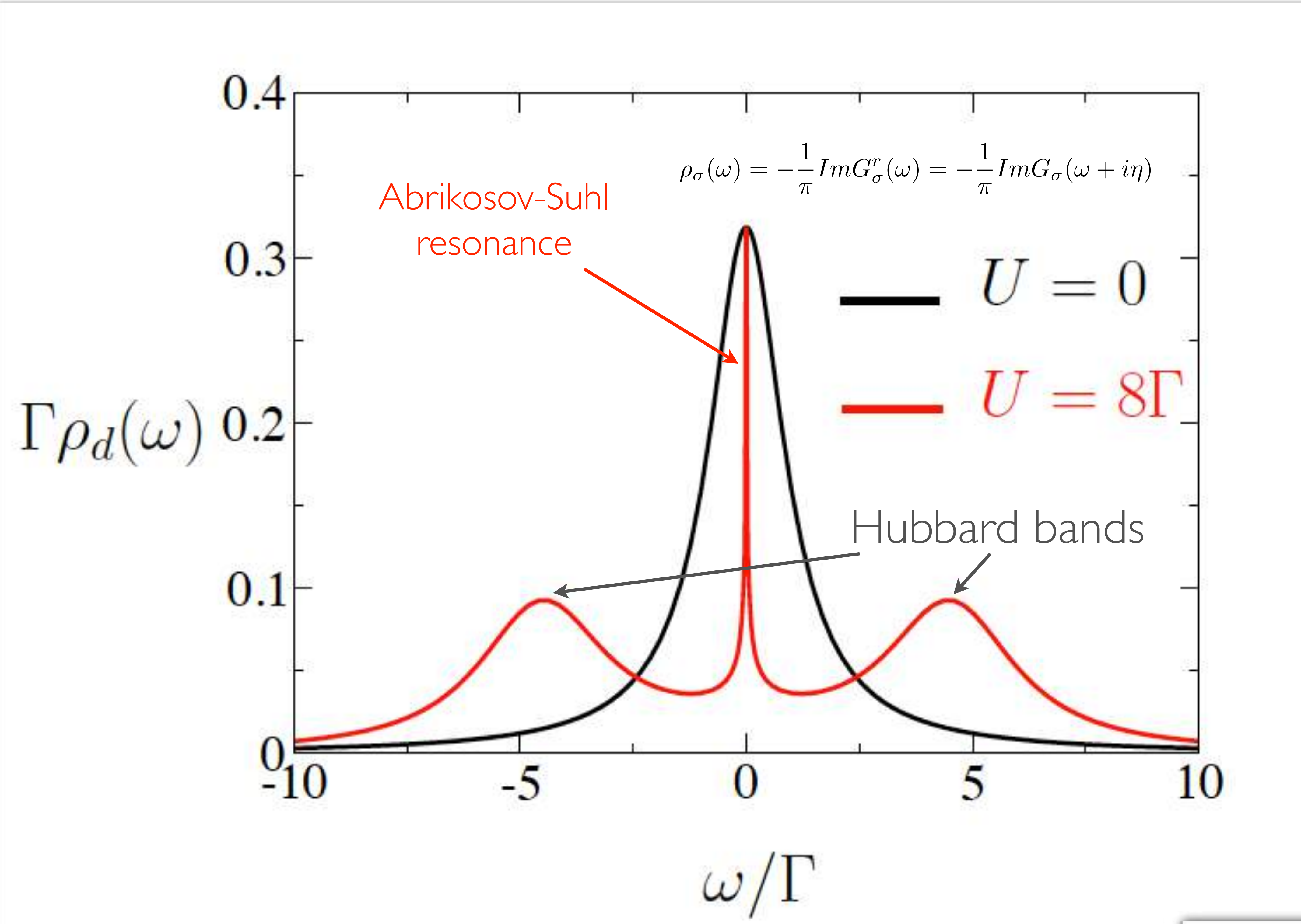
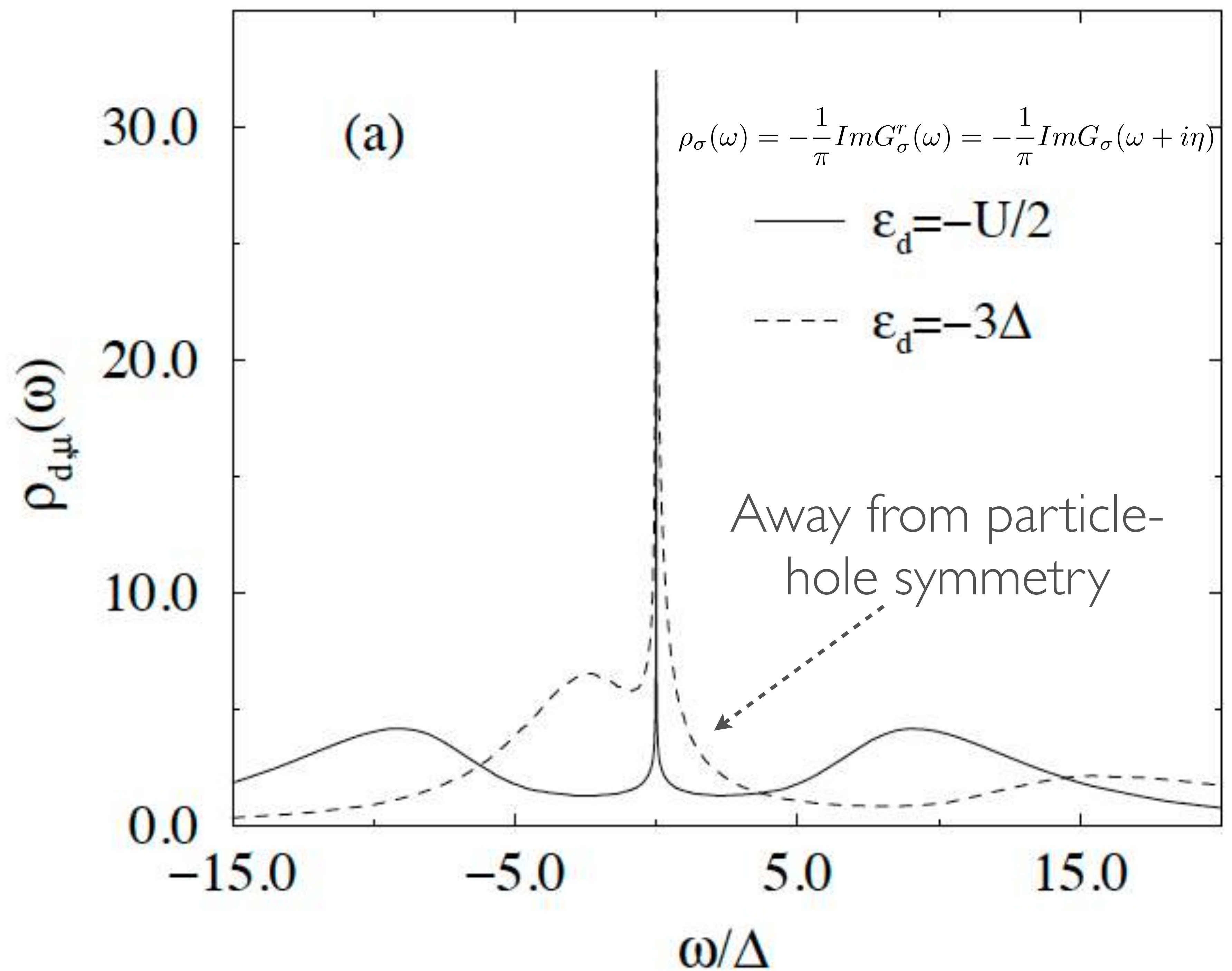
How about **dynamics**?



NRG calculations: Frota & Oliveira 86, Sakai, Shimizu & Kasuya 89, Costi & Hewson 90)

How about **dynamics**?



NRG calculations: Frota & Oliveira 86, Sakai, Shimizu & Kasuya 89, Costi & Hewson 90)

$$\rho_\sigma(\omega) = -\frac{1}{\pi} Im G^r_\sigma(\omega) = -\frac{1}{\pi} Im G_\sigma(\omega + i\eta)$$

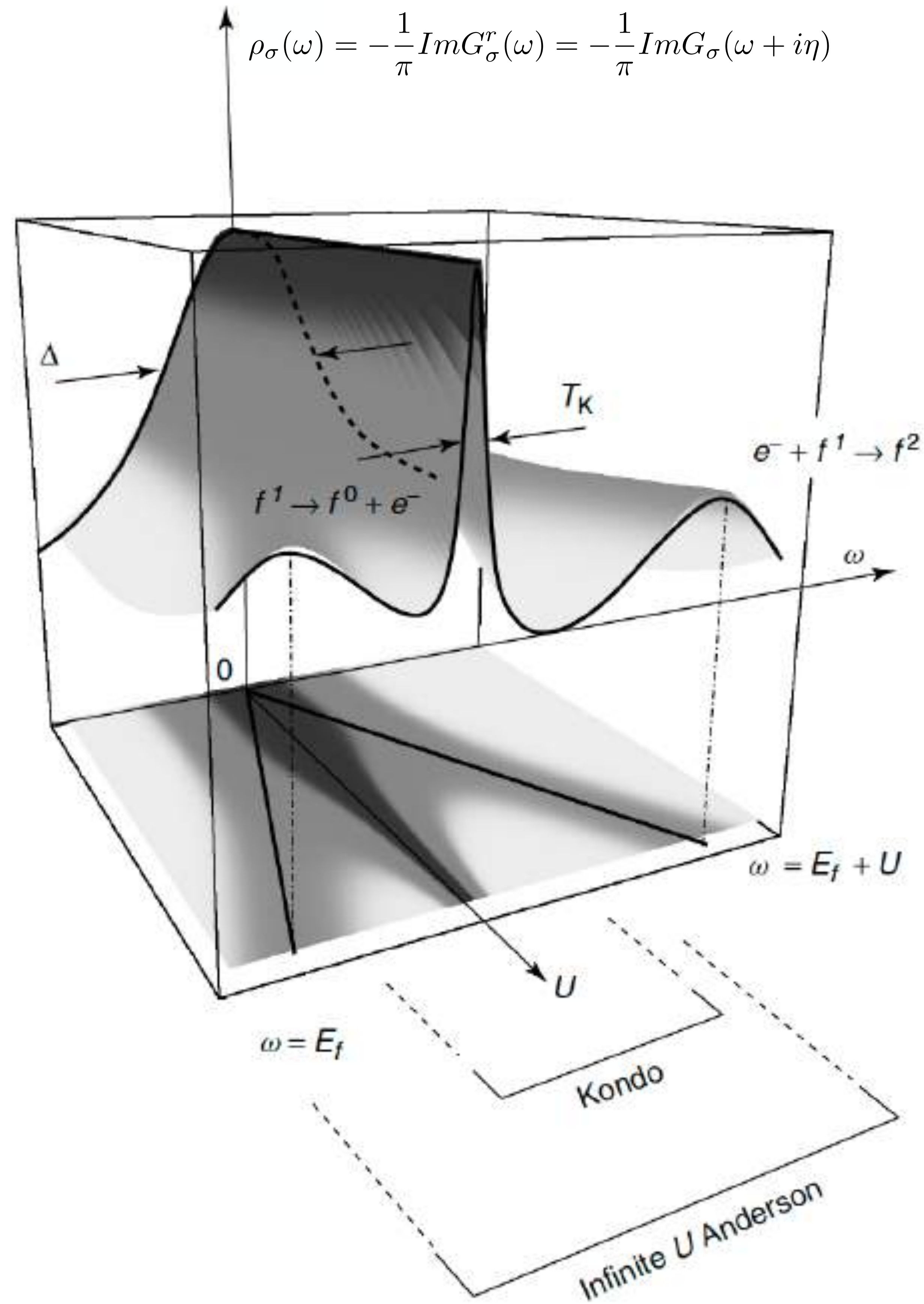
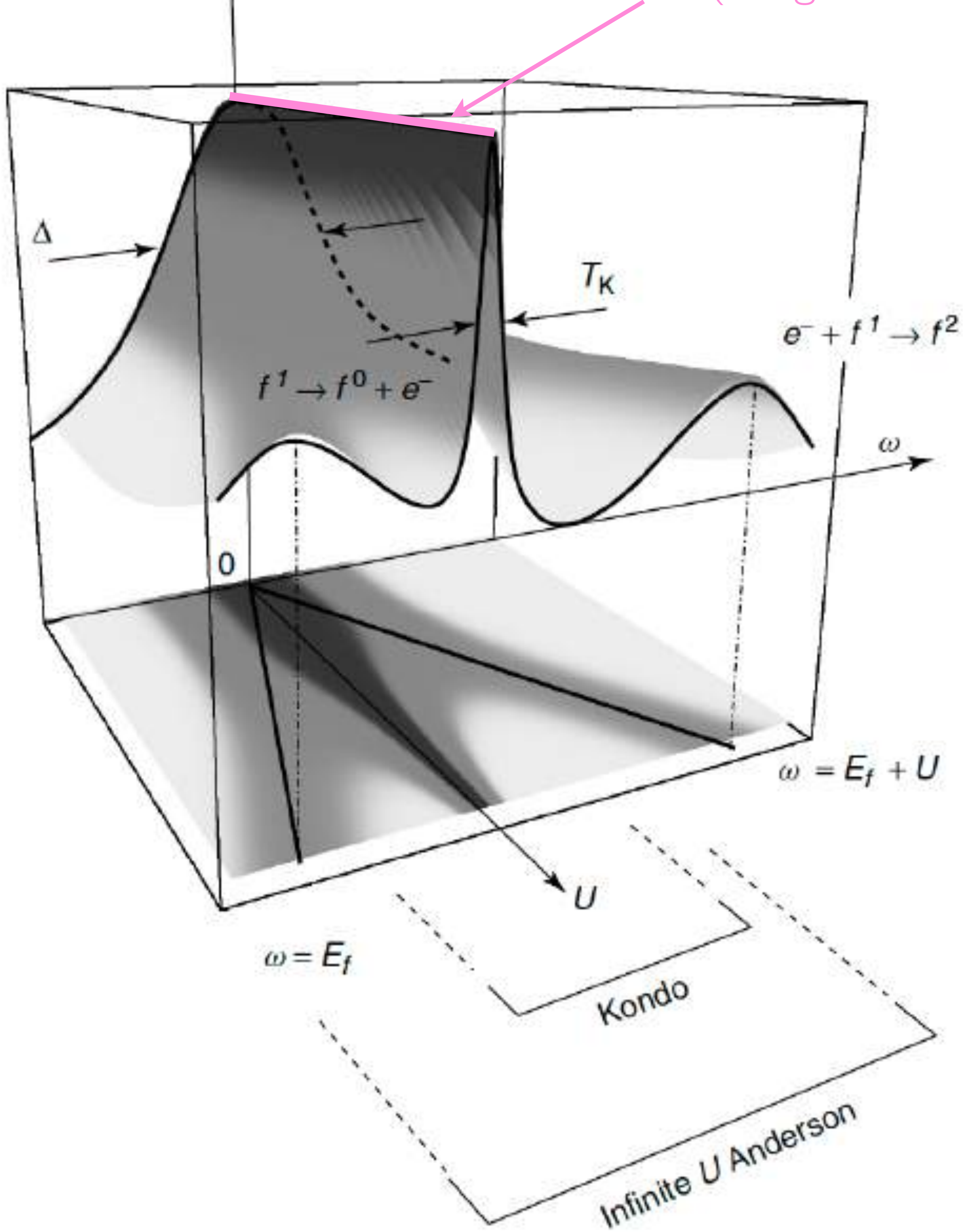


Image Piers Coleman, Rutgers

$$\rho_\sigma(\omega) = -\frac{1}{\pi} Im G^r_\sigma(\omega) = -\frac{1}{\pi} Im G_\sigma(\omega + i\eta)$$

Adiabatic Invariant (Langreth 1966)



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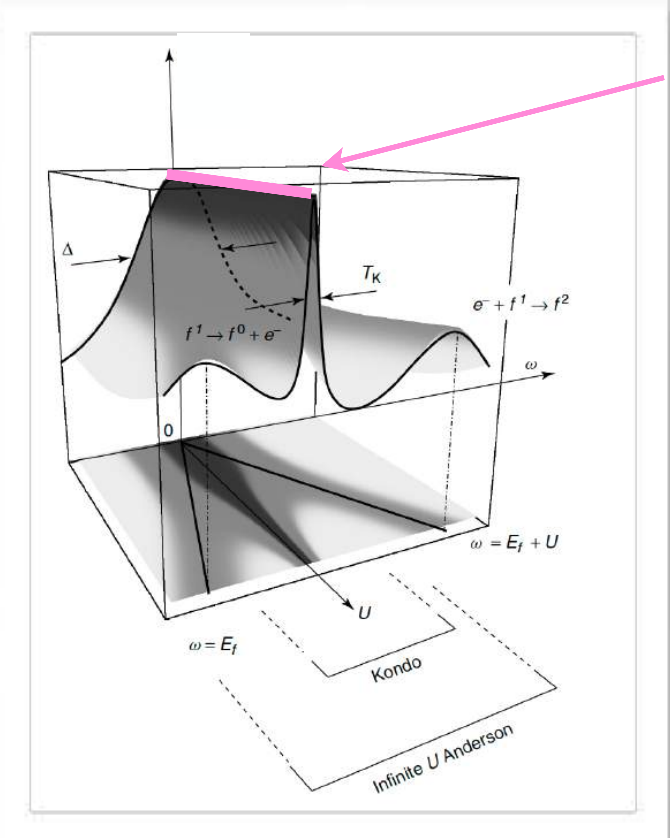


Adiabatic Invariant (Langreth 1966)

For large U we expect the two Hubbard bands, since the spectral weight is conserved each band should contribute 1/2.

$$\int A(\omega) d\omega = 1$$

Remarkably, the spectral function at $\omega = 0$ remains invariant as the interaction increases (always equal to the non-interacting value)

$$A(\omega = 0) = \frac{1}{\pi\Gamma} sin^2\delta$$

Deep result: the spectral function must always contain a peak of height $\frac{1}{\pi\Gamma} sin^2\delta$

and vanishingly small weight Z<<1 as U increases. This narrow resonance is a direct consequence of local Fermi liquid behaviour!

$$Z \sim \frac{T_K}{\Gamma}$$

Fermi liquid picture

Langreth Physical Review 150, 516, 1966: Friedel Sum rule for the Anderson model for arbitrary interaction.

Exact relations (Fermi-liquid) for the self-energy at T=0:

$$\Sigma_\sigma(\omega \pm i\eta) = \Sigma_\sigma^R(\omega) \mp i\Sigma_\sigma^I(\omega)$$

$$\Sigma_\sigma^I(\varepsilon_F) = 0$$

$$\Sigma_\sigma^I(\omega) \propto \omega^2 \quad \omega \to \varepsilon_F$$

$$Im \int_{-\infty}^{\varepsilon_F} \frac{\partial \Sigma_\sigma(\omega)}{\partial \omega} G_\sigma(\omega) d\omega = 0$$

Fermi liquid picture

Langreth Physical Review 150, 516, 1966: Friedel Sum rule for the Anderson model for arbitrary interaction.

Exact relations (Fermi-liquid) for the self-energy at T=0:

$$\frac{1}{\omega - \varepsilon_d + i\Gamma - \Sigma(\omega) + i\eta} = \frac{\partial}{\partial\omega} ln(\omega - \varepsilon_d + i\Gamma - \Sigma(\omega) + i\eta) + \frac{\partial\Sigma(\omega)/\partial\omega}{\omega - \varepsilon_d + i\Gamma - \Sigma(\omega) + i\eta}$$

Fermi liquid picture

Langreth Physical Review 150, 516, 1966: Friedel Sum rule for the Anderson model for arbitrary interaction.

Exact relations (Fermi-liquid) for the self-energy at T=0:

$$Im\int_{-\infty}^{\varepsilon_F}\frac{\partial\Sigma_\sigma(\omega)}{\partial\omega}G_\sigma(\omega)d\omega=0$$

If we integrate the density of states to get the occupation

$$Im\int\frac{1}{\omega-\varepsilon_d+i\Gamma-\Sigma(\omega)+i\eta}=Im\int\frac{\partial}{\partial\omega}ln(\omega-\varepsilon_d+i\Gamma-\Sigma(\omega)+i\eta)+Im\int\frac{\partial\Sigma(\omega)/\partial\omega}{\omega-\varepsilon_d+i\Gamma-\Sigma(\omega)+i\eta}$$

$$\langle n_\sigma\rangle=\frac{1}{2}-\frac{1}{\pi}arctan^{-1}(\frac{\varepsilon_d-\varepsilon_F+\Sigma^R_\sigma(\varepsilon_F)+\Sigma^I_\sigma(\varepsilon_F)}{\Gamma})$$

Fermi liquid picture

Langreth Physical Review 150, 516, 1966: Friedel Sum rule for the Anderson model for arbitrary interaction.

Exact relations (Fermi-liquid) for the self-energy at T=0:

$$\langle n_\sigma \rangle = \frac{1}{2} - \frac{1}{\pi} arctan^{-1}(\frac{\varepsilon_d - \varepsilon_F + \Sigma^R_\sigma(\varepsilon_F)}{\Gamma}) = \frac{\delta_\sigma(\varepsilon_F)}{\pi}$$

$$\Downarrow$$

$$\rho_\sigma(\varepsilon_F) = \frac{1}{\pi\Gamma} sin^2\delta_\sigma(\varepsilon_F) = \frac{1}{\pi\Gamma} sin^2(\pi\langle n_\sigma \rangle)$$

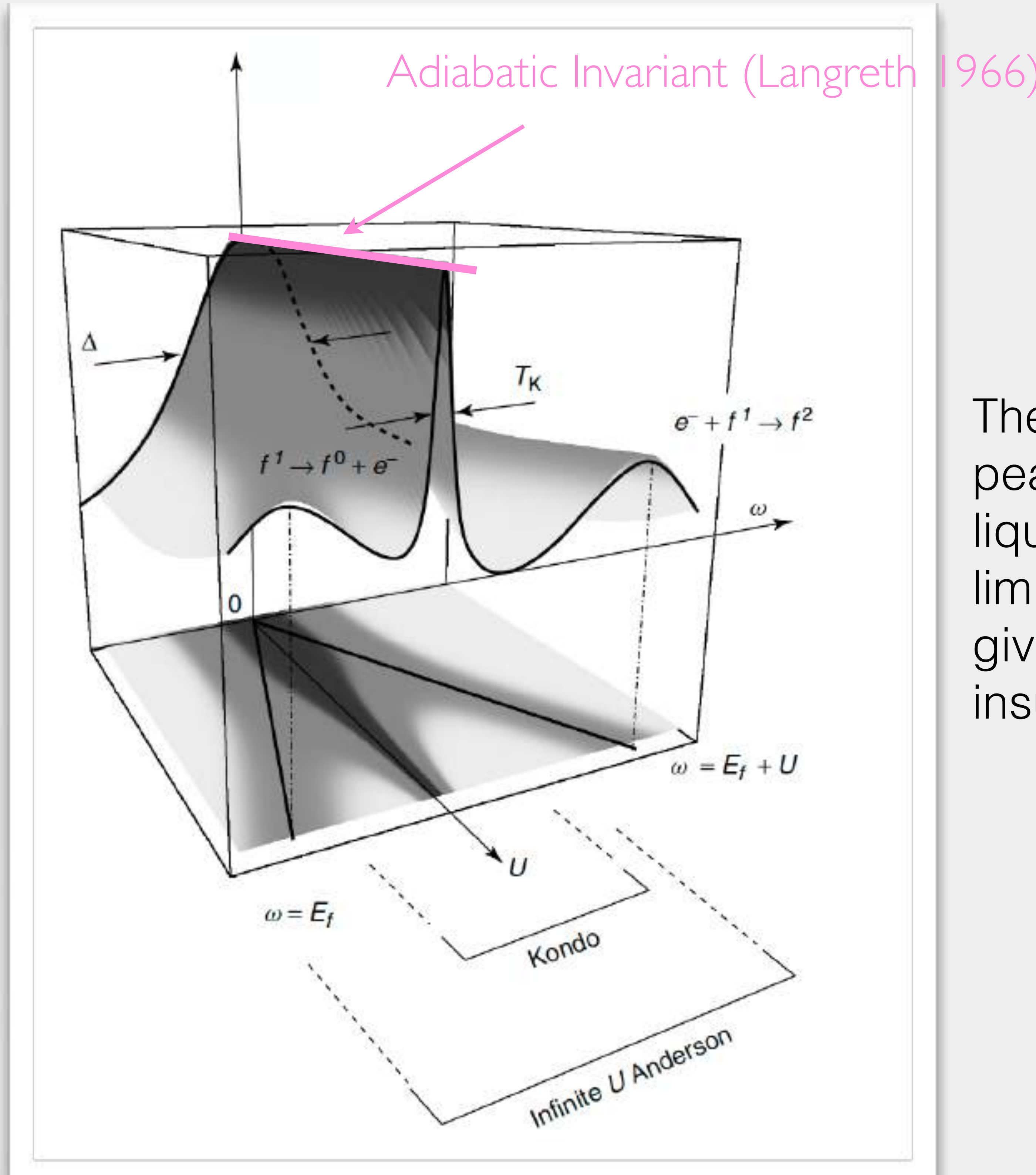
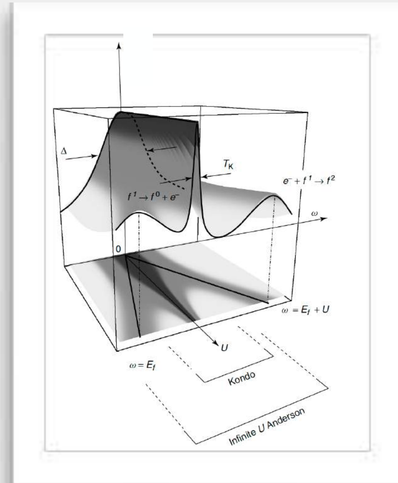
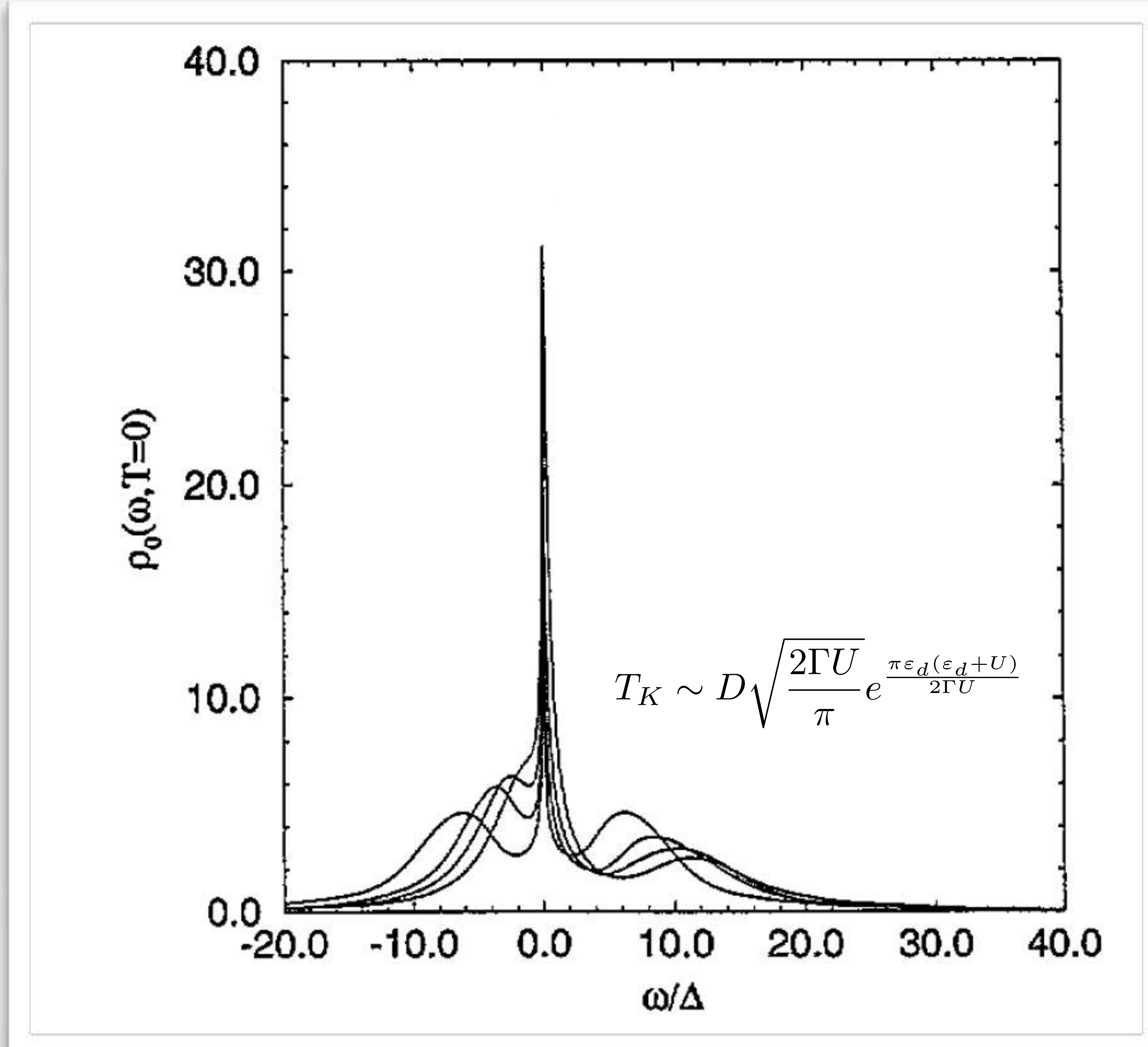


Image Piers Coleman, Rutgers

The Abrikosov-Suhl resonance (or “Kondo peak”) is a direct consequence of Fermi liquid behaviour in the strong coupling limit. This physics is similar as the one giving the “coherence peaks” in Mott insulators (Leni’s lecture)

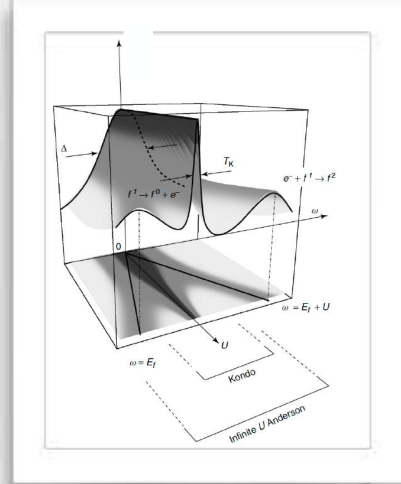
Abrikosov-Suhl resonance

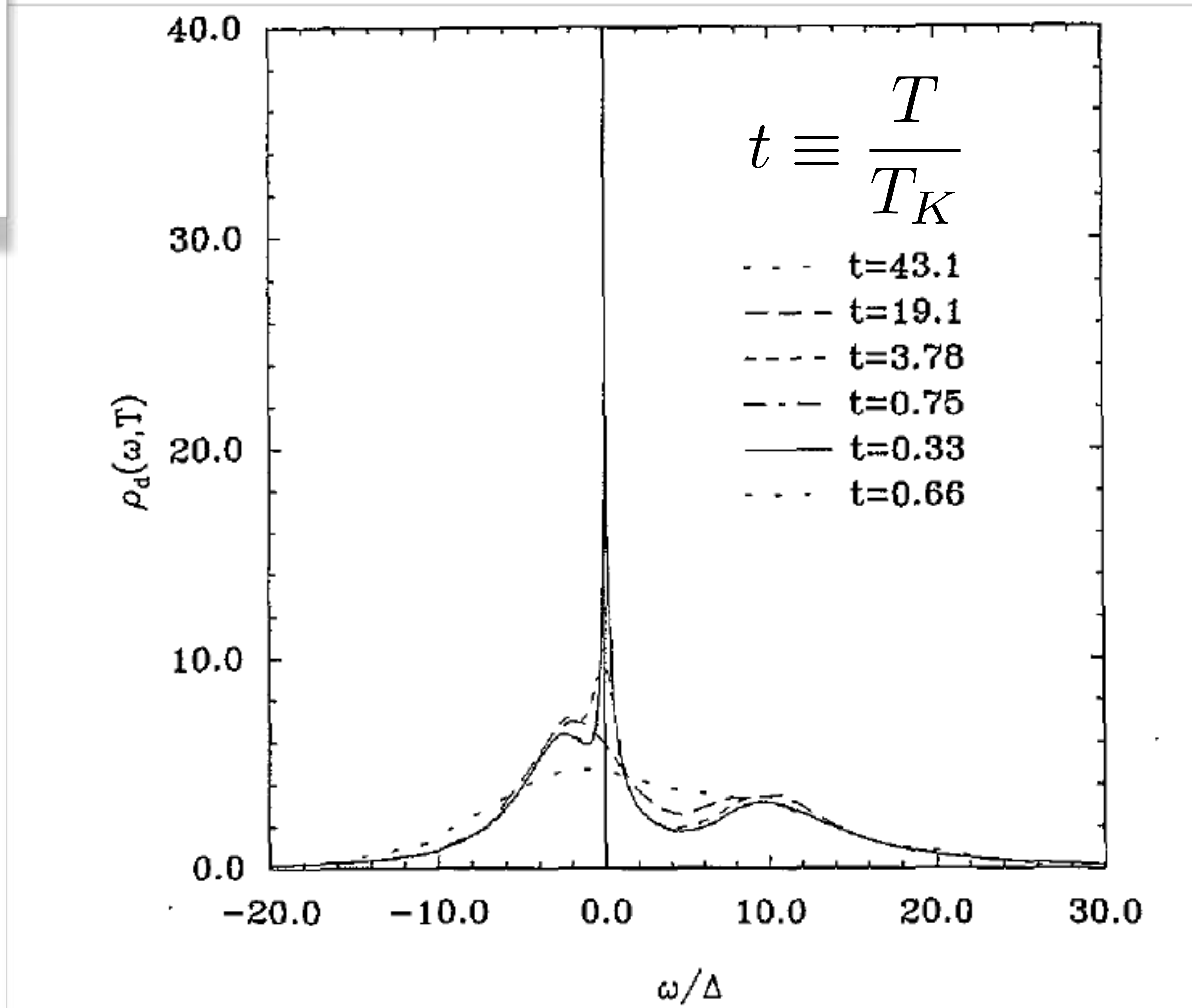




Level position

Abrikosov-Suhl resonance

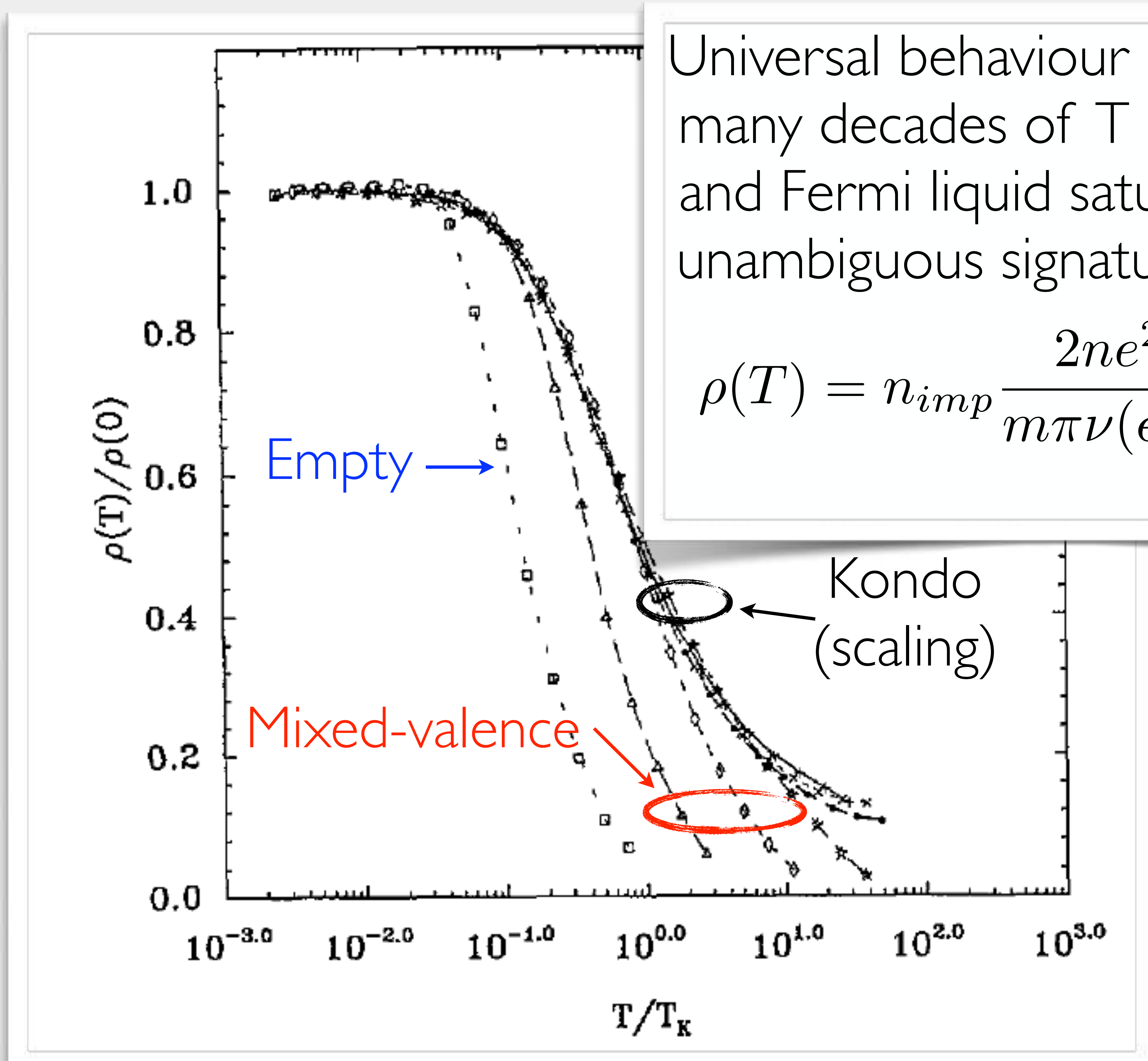




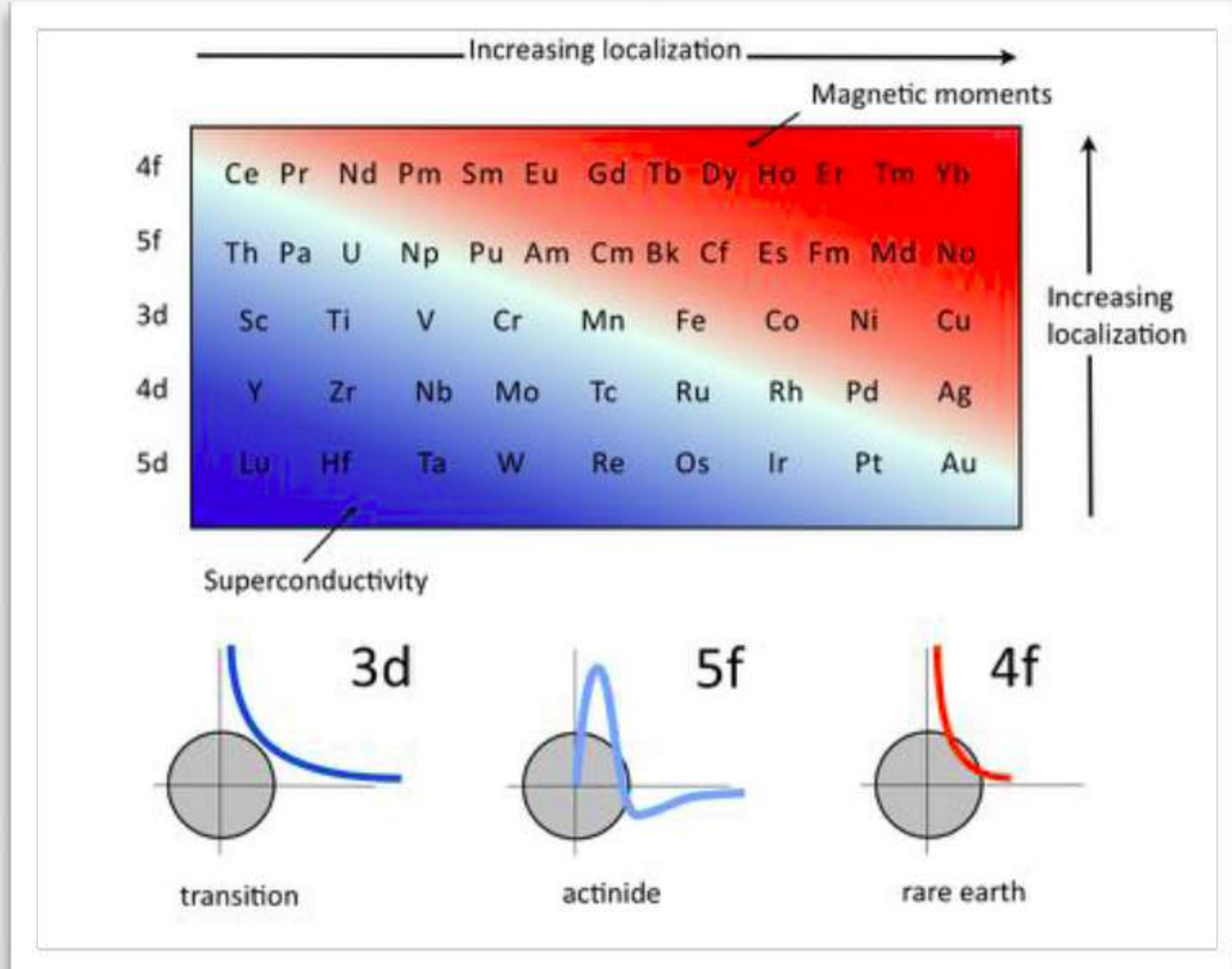
Temperature dependence

Universal behaviour (scaling) over many decades of T (logarithmic) and Fermi liquid saturation is the unambiguous signature of Kondo

$$\rho(T) = n_{imp}\frac{2ne^2}{m\pi\nu(\epsilon_F)}F(\frac{T}{T_K})$$



Heavy fermion materials: strong correlations



- In the periodic table, the most strongly interacting electrons reside in orbitals that are well localised.
- The properties of heavy-fermion compounds derive from the partially filled f orbitals of rare-earth or actinide ions.

Heavy fermion materials: strong correlations

- Heavy-fermion materials display properties which change qualitatively (unconventional superconductivity, quantum criticality, etc), depending on the temperature, so much so, that **the room-temperature and low-temperature behavior almost resembles two different materials.**

Type	Material	T^* (K)	$T_c,\ x_c,\ B_c$	Properties	ρ	$\mathrm{mJ\,mol^{-1}K^{-2}}$ γ_n	References
Metal	$CeCu_6$	10	–	Simple HF metal	T^2	1600	Stewart, Fisk and Wire (1984a) and Onuki and Komatsubara (1987)
Super-conductors	$CeCu_2Si_2$	20	$T_c = 0.17\,\mathrm{K}$	First HFSC	T^2	800–1250	Steglich *et al.* (1976) and Geibel *et al.* (1991a,b)
	UBe_{13}	2.5	$T_c = 0.86\,\mathrm{K}$	Incoherent metal→HFSC	$\rho_c \sim 150\,\mu\Omega\,\mathrm{cm}$	800	Ott, Rudigier, Fisk and Smith (1983, 1984)
	$CeCoIn_5$	38	$T_c = 2.3$	Quasi 2D HFSC	T	750	Petrovic *et al.* (2001) and Sidorov *et al.* (2002)
Kondo insulators	$Ce_3Pt_4Bi_3$	$T_\chi \sim 80$	–	Fully gapped KI	$\sim e^{\Delta/T}$	–	Hundley *et al.* (1990) and Bucher, Schlessinger, Canfield and Fisk (1994)
	CeNiSn	$T_\chi \sim 20$	–	Nodal KI	Poor metal	–	Takabatake *et al.* (1990, 1992) and Izawa *et al.* (1999)
Quantum critical	$CeCu_{6-x}Au_x$	$T_0 \sim 10$	$x_c = 0.1$	Chemically tuned QCP	T	$\sim \frac{1}{T_0} \ln\left(\frac{T_0}{T}\right)$	von Löhneysen *et al.* (1994) and von Löhneysen (1996)
	$YbRh_2Si_2$	$T_0 \sim 24$	$B_\perp = 0.06\,\mathrm{T}$ $B_\parallel = 0.66\,\mathrm{T}$	Field-tuned QCP	T	$\sim \frac{1}{T_0} \ln\left(\frac{T_0}{T}\right)$	Trovarelli *et al.* (2000), Paschen *et al.* (2004), Custers *et al.* (2003) and Gegenwart *et al.* (2005)
SC + other order	UPd_2Al_3	110	$T_{AF} = 14\,\mathrm{K}$, $T_{sc} = 2\,\mathrm{K}$	AFM + HFSC	T^2	210	Geibel *et al.* (1991a), Sato *et al.* (2001) and Tou *et al.* (1995)
	URu_2Si_2	75	$T_1 = 17.5\,\mathrm{K}$, $T_{sc} = 1.3\,\mathrm{K}$	Hidden order and HFSC	T^2	120/65	Palstra *et al.* (1985) and Kim *et al.* (2003)

Unless otherwise stated, T^* denotes the temperature of the maximum in resistivity. T_c, x_c, and B_c denote critical temperature, doping, and field. ρ denotes the temperature dependence in the normal state. $\gamma_n = C_V/T$ is the specific heat coefficient in the normal state.

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Heavy fermion materials: strong correlations

- The first heavy-electron materials to be discovered are now called Kondo insulators.
- In the late 1960s, an unusual metal, SmB6, containing magnetic Sm^{3+} ions was discovered . While apparently a magnetic metal with a Curie–Weiss susceptibility at room temperature, on cooling SmB6 transforms continuously into a paramagnetic insulator **with a tiny 10 meV gap.**
- The first heavy-fermion metal, $CeAl_3$ was discovered in the mid 1970s.

Heavy fermion metals

Transport properties

- Curie-Weiss susceptibility at high T.
- Paramagnetic spin susceptibility at low T
- Quadratic temperature dependence of the low temperature resistivity.
- A dramatic enhancement of the linear specific heat (e.g. for $CeAl_3$ more than 1500 times that of Copper!).

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Heavy fermion metals

- These transport properties suggest that Kondo physics is relevant. If this is correct, the resulting Fermi liquid at low temperatures is composed of quasiparticles with greatly enhanced masses.

↓

Heavy fermions

Heavy fermion metals

- Andres, Graebner, and Ott proposed in their 1975 paper that the ground-state excitations of CeAl3 were those of a *Landau Fermi-liquid*, in which the effective mass of the quasiparticles is about 1000 bare electron masses!
- Like other cerium heavy-fermion materials, the cerium atoms in this metal are in a $Ce^{3+}(4f^1)$ configuration, and because they are spin–orbit coupled, they form huge local moments with a spin of $J = 5/2$.
- In their paper, Andres, Ott, and Graebner suggested that a **lattice version of the Kondo effect** is responsible.

VOLUME 35, NUMBER 26 PHYSICAL REVIEW LETTERS 29 DECEMBER 1975

4f-Virtual-Bound-State Formation in $CeAl_3$ at Low Temperatures

K. Andres and J. E. Graebner
Bell Laboratories, Murray Hill, New Jersey 07974

and

H. R. Ott
Laboratorium für Festkörperphysik, Eidgenössische Technische Hochschule, Hönggerberg, Zürich, Switzerland

(Received 25 August 1975)

Specific-heat and electrical-resistivity measurements in $CeAl_3$ below 0.2 K reveal enormous magnitudes of the linear specific-heat term $C=\gamma T$ (γ=1620 mJ mole/K^2) and the T^2 term in $\rho=AT^2$ (A=35 $\mu\Omega$ cm/K^2). We conclude that the 4f electrons obey Fermi statistics at low temperatures because of the formation of virtual bound 4f states.

Heavy fermion materials

- High temperatures: local 4f or 5f moments

Low lying magnetic multiplet

$$N = 2j + 1$$

For example Ce^{3+} $|4f^1 : j, m\rangle$

$$L = 3, S = 1/2$$

$$J = L - S = 5/2$$

$$N = 6$$

Remember, local moments have a Curie spin susceptibility

$$\chi = \frac{(g_J \mu_B)^2 J(J+1)}{3k_B T}$$

$$S = k_B ln(2J + 1)$$ Large unquenched entropy

$S = k_B ln(2J+1)$

Heavy fermion materials

The entropy can also be written as an integral of the specific heat

$$S = \int_0^T \frac{C_V}{T'} dT'$$

At low temperature, the Kondo effect develops and the local moments become quenched. This implies that the spin entropy is rapidly lost from the material.

This rapid loss of spin entropy forces a sudden rise in the specific heat

$$\gamma = Lim_{T\rightarrow 0} \frac{C_V}{T} = \frac{\pi^2 k_B^2}{3} \rho^*$$ Sommerfeld coefficient

$$\rho^* = \frac{k_F m^*}{\pi^2 \hbar^2}$$

Huge increase of effective mass at low temperatures (hence the name "Heavy Fermions")

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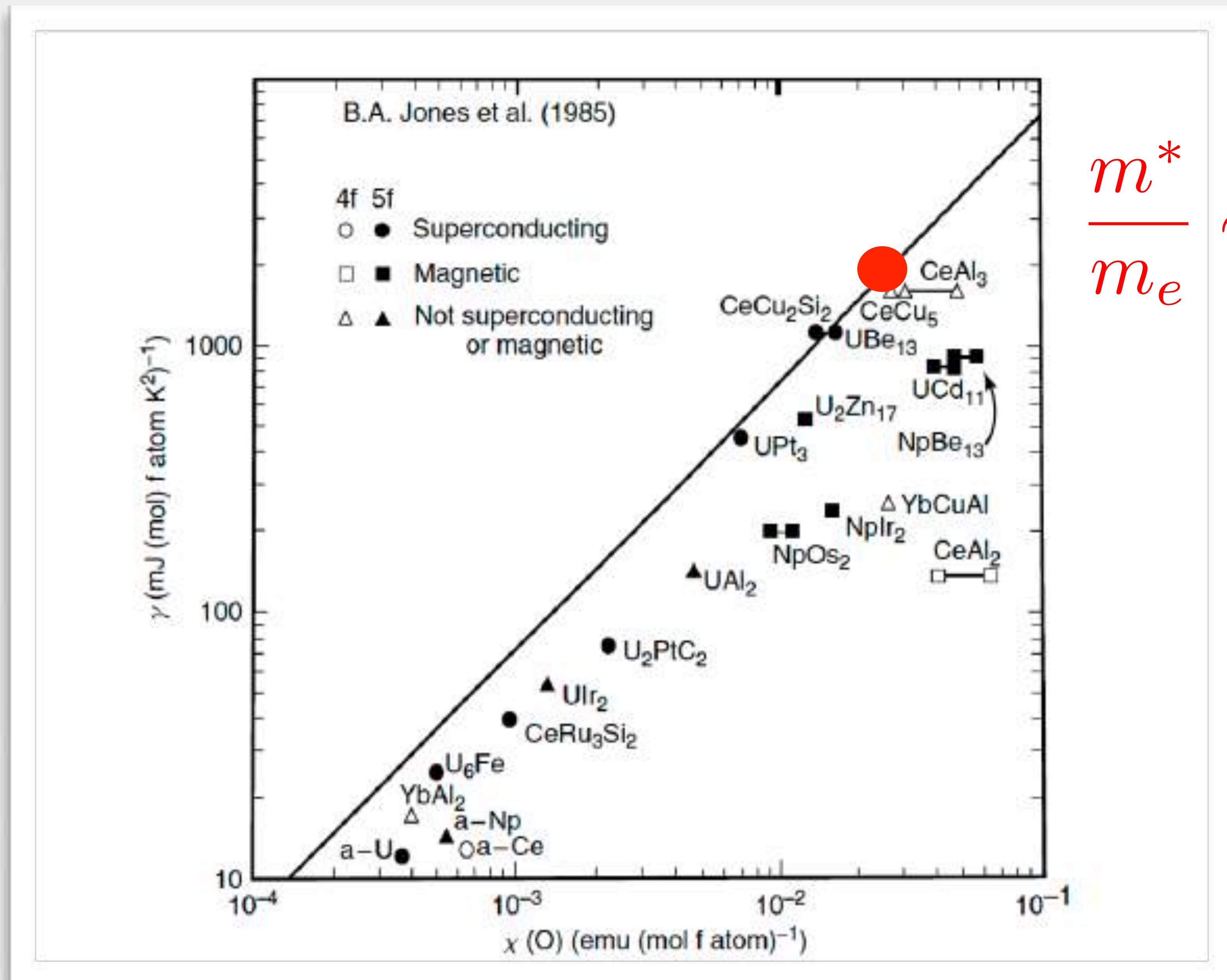
Heavy fermion materials

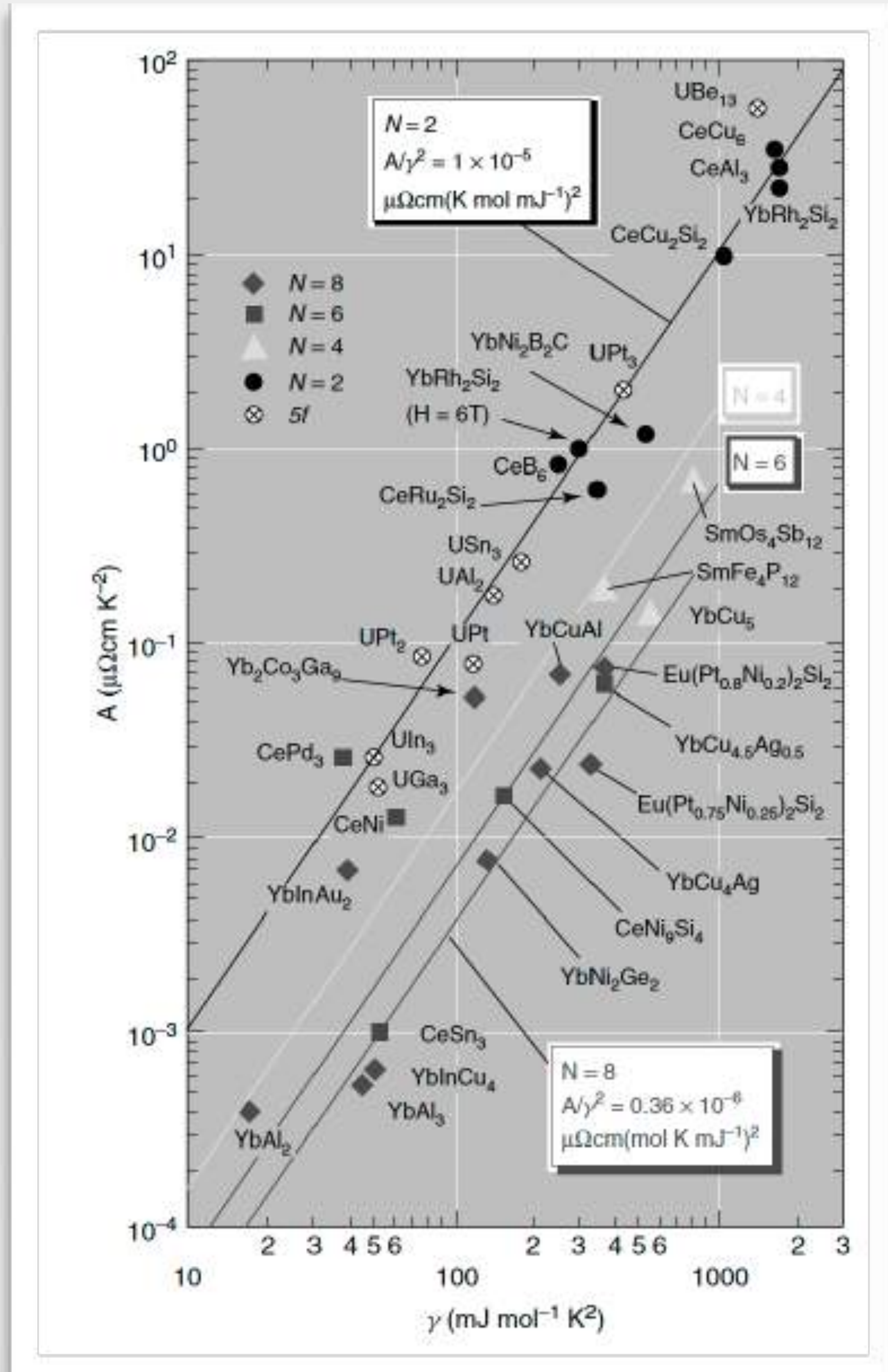
$$\rho^* = \frac{k_F m^*}{\pi^2 \hbar^2}$$

Huge increase of effective mass at low temperatures (hence the name "Heavy Fermions")



$$\frac{m^*}{m_e} \sim 1000!!$$

Heavy fermion materials



Further confirmation of the Fermi-liquid behavior of heavy-fermion systems is obtained when the Sommerfeld coefficient of the linear term of the specific heat is compared with the coefficient A of the resistivity

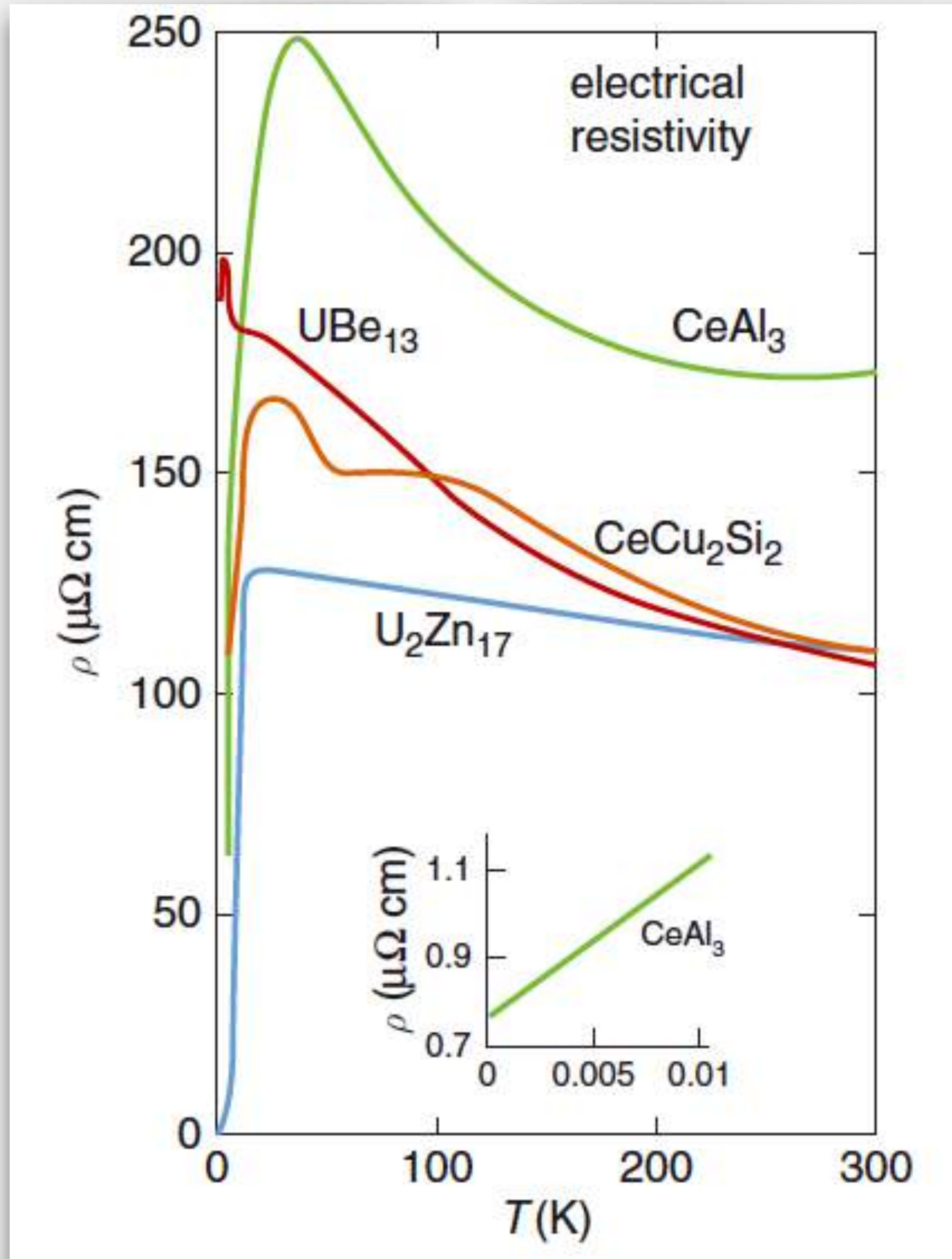
$$\rho = \rho_0 + AT^2$$

$$\left.\begin{array}{l} \gamma \sim m^* \\ A \sim (m^*)^2 \end{array}\right\} \frac{A}{\gamma^2} \sim cons$$

Kadowaki-Woods

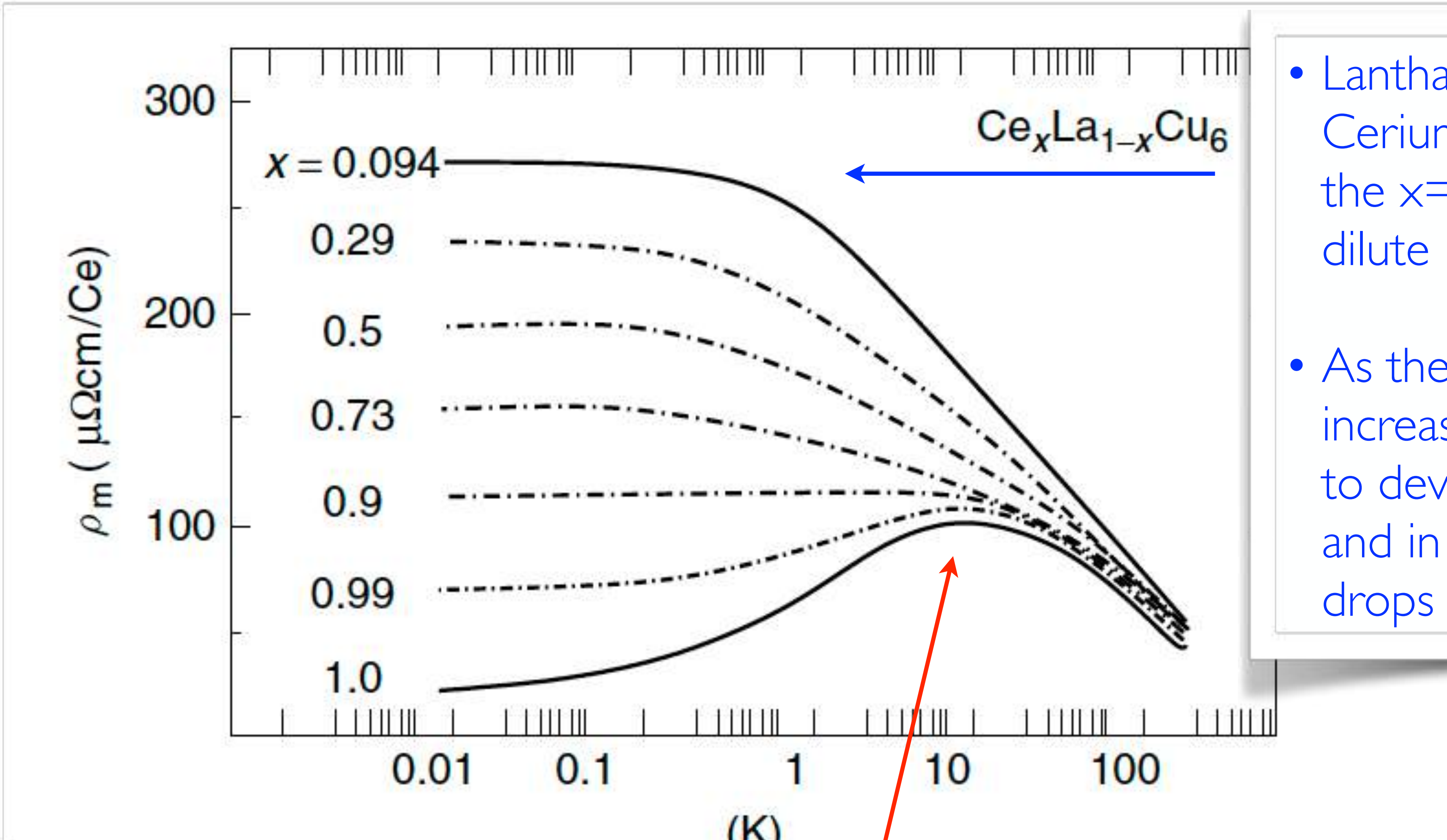
Heavy fermion insulators

Transport properties



- While apparently a magnetic metal with a Curie–Weiss susceptibility at room temperature, on cooling these materials they transform continuously into a paramagnetic insulator with very tiny gaps (around 10 meV).

Development of coherence in heavy fermion systems



- Lanthanum is iso-electronic with Cerium but has an empty f-shell so the x=0 limit corresponds to a dilute Kondo system.
- As the concentration of Cerium increases, the resistivity curve starts to develop a coherence maximum and in the concentrated limit it drops to zero as a Fermi liquid.

Development of Coherence

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How to explain all this?

This experimental evidence suggests that heavy fermion materials can be understood as a lattice version of the Kondo effect with a renormalised density of states

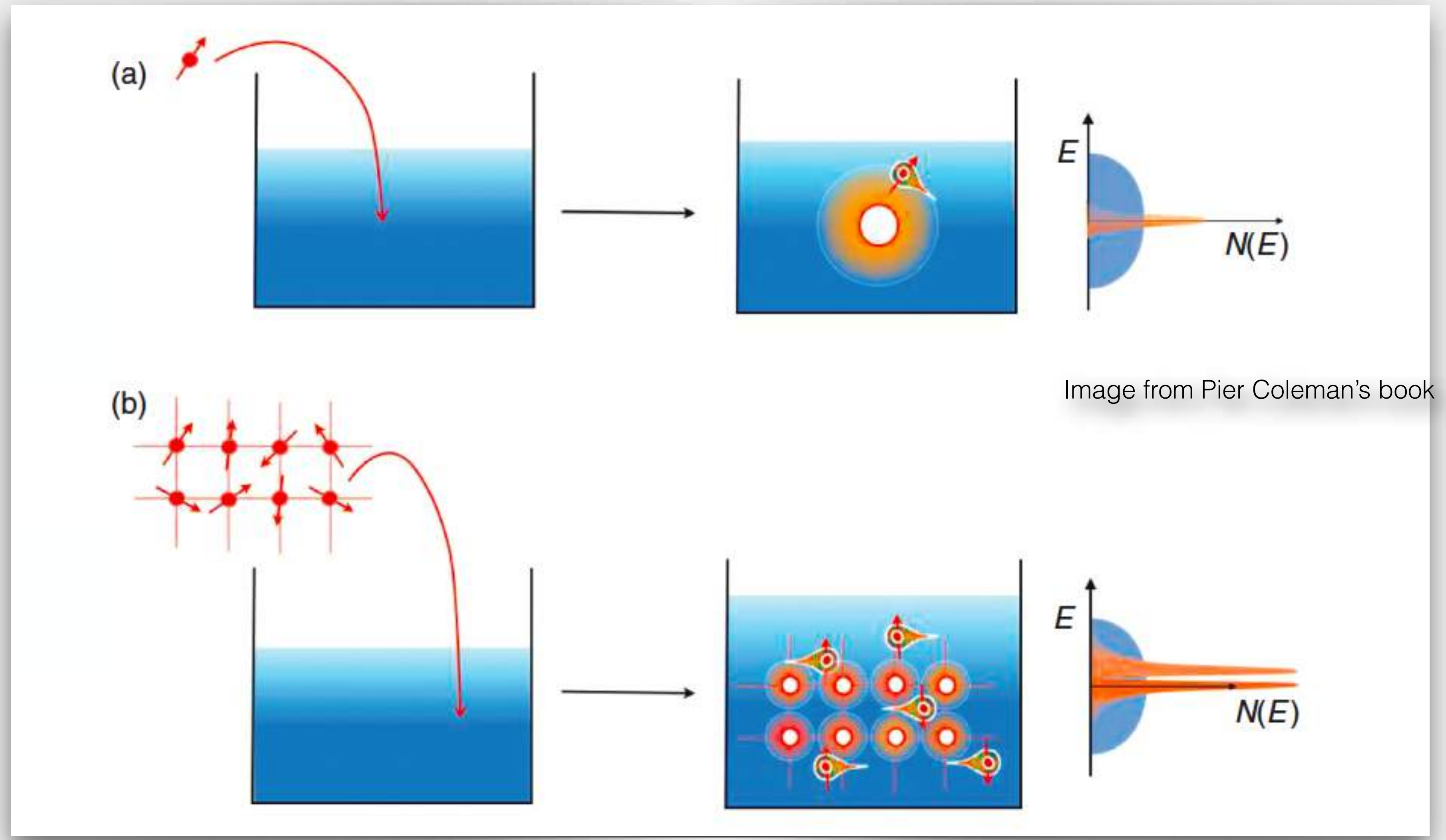


Image from Pier Coleman's book

Immersion of a lattice of spins in a conduction sea injects a resonance at each site in the lattice, giving rise to a **new band of delocalized heavy fermions** with a hybridization gap. The density of carriers is increased in the Kondo lattice.

Heavy fermion superconductors

- The early resistance to this Kondo explanation was rooted in a number of misconceptions about spin physics and the Kondo effect. Some of the first heavy-electron systems are superconductors, e.g. UBe_{13} , yet it was well known that small concentrations of magnetic ions, typically a few percent, suppress conventional superconductivity, so the appearance of superconductivity in a dense magnetic system appeared at first sight to be impossible!!!

- How can be explain heavy-fermion superconductors?: the Kondo effect quenches the local moments to form a new kind of heavy-fermion metal.

Heavy fermion materials

Transport properties

• High temperatures: heavy fermion compounds exhibit a large saturated resistivity, induced by incoherent spin-flip scattering of the conduction electrons of the local f moments.

• Low temperatures: Quenching of local moments (Kondo-like) together with development of phase coherence.

The simplest model which might be capable of describing heavy-fermion, mixed valence, and Kondo behavior depending on the values of the parameters is the **periodic Anderson model** (Varma and Yafet, Phys. Rev. B 13, 2950, 1976)

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{i,\sigma} \varepsilon_f f^\dagger_{i,\sigma} f_{i,\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} +$$

$$\sum_{i,k,\sigma} (V_k e^{-ik.R_i} c^\dagger_{k,\sigma} f_{i,\sigma} + V^*_k e^{ik.R_i} f^\dagger_{i,\sigma} c_{k,\sigma})$$

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{i,\sigma} \varepsilon_f f^\dagger_{i,\sigma} f_{i,\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} +$$
$$\sum_{i,k,\sigma} (V_k e^{-ik.R_i} c^\dagger_{k,\sigma} f_{i,\sigma} + V_k^* e^{ik.R_i} f^\dagger_{i,\sigma} c_{k,\sigma})$$

Non-interacting case

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \varepsilon_f f^\dagger_{k,\sigma} f_{k,\sigma} +$$

Bloch representation

$$\sum_{k,\sigma} (V_k c^\dagger_{k,\sigma} f_{k,\sigma} + V_k^* f^\dagger_{k,\sigma} c_{k,\sigma})$$

$$f^\dagger_{k,\sigma} = \sum_j e^{ikR_j} f^\dagger_{j,\sigma}$$ Etc

$$H=\sum_{k,\sigma}\varepsilon_k c^\dagger_{k,\sigma}c_{k,\sigma}+\sum_{i,\sigma}\varepsilon_f f^\dagger_{i,\sigma}f_{i,\sigma}+\sum_i U n_{i\uparrow}n_{i\downarrow}+$$
$$\sum_{i,k,\sigma}(V_k e^{-ik.R_i}c^\dagger_{k,\sigma}f_{i,\sigma}+V_k^* e^{ik.R_i}f^\dagger_{i,\sigma}c_{k,\sigma})$$

Non-interacting case

$$H=\sum_{k,\sigma}\varepsilon_k c^\dagger_{k,\sigma}c_{k,\sigma}+\sum_{k,\sigma}\varepsilon_f f^\dagger_{k,\sigma}f_{k,\sigma}+$$

Bloch representation

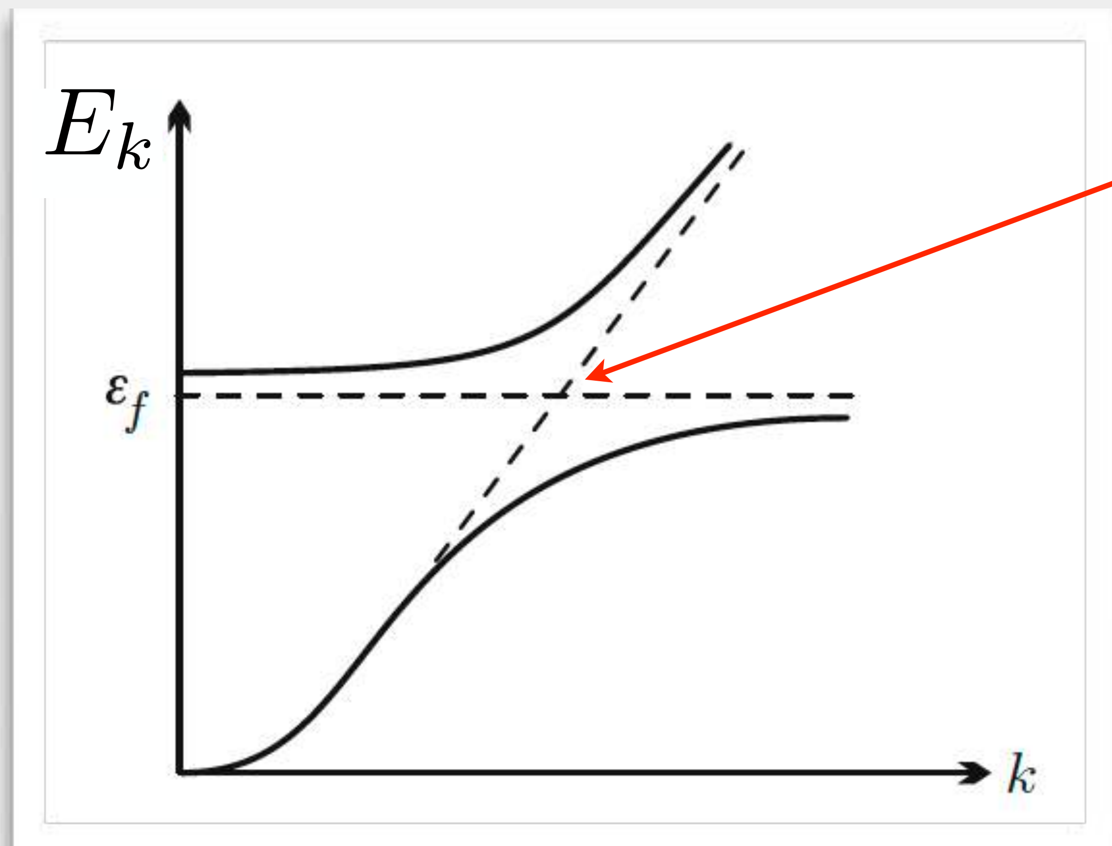
$$\sum_{k,\sigma}(V_k c^\dagger_{k,\sigma}f_{k,\sigma}+V_k^* f^\dagger_{k,\sigma}c_{k,\sigma})$$

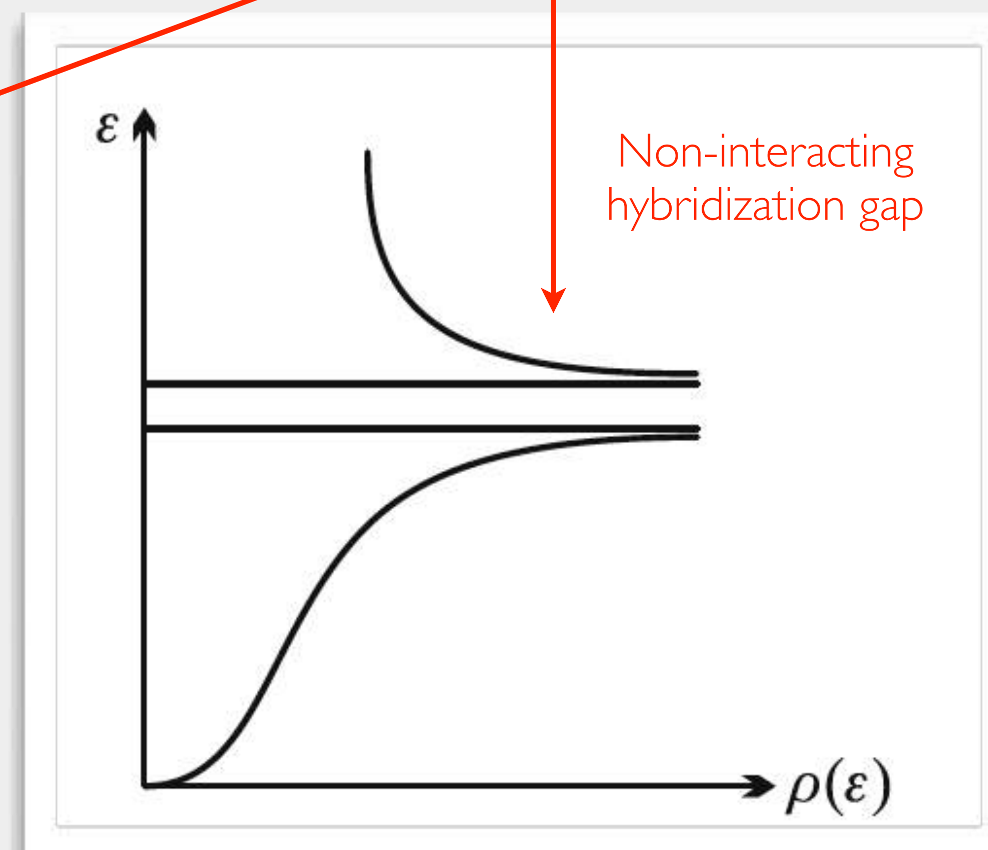
$$\left.\begin{array}{l}\alpha^{(+)}_{k,\sigma}=u_k c_{k,\sigma}+v_k f_{k,\sigma}\\ \alpha^{(-)}_{k,\sigma}=-v_k c_{k,\sigma}+u_k f_{k,\sigma}\end{array}\right\} \quad \begin{array}{l}|u_k|^2=\frac{1}{2}[1+\frac{\varepsilon_k-\varepsilon_f}{\sqrt{(\varepsilon_k-\varepsilon_f)^2+4|V_k|^2}}]\\ |v_k|^2=\frac{1}{2}[1-\frac{\varepsilon_k-\varepsilon_f}{\sqrt{(\varepsilon_k-\varepsilon_f)^2+4|V_k|^2}}]\end{array}$$

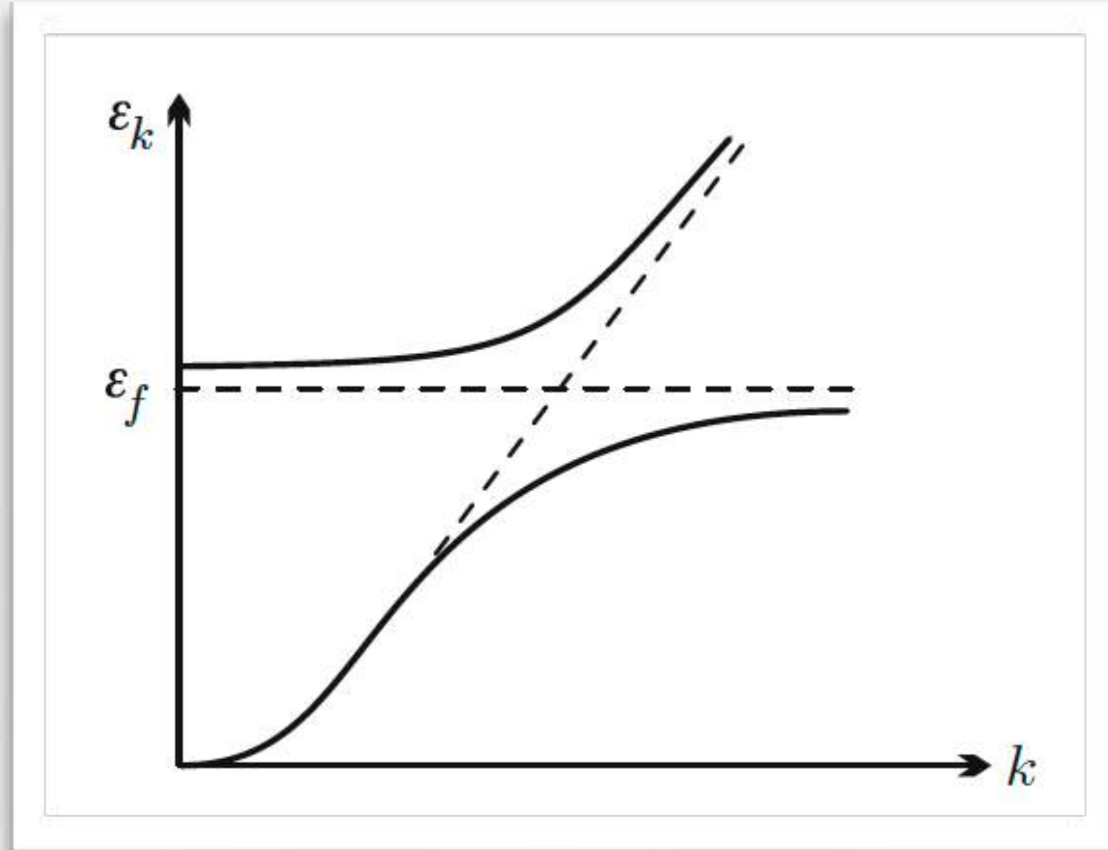
$$E_k^{\pm}=\frac{1}{2}(\varepsilon_k+\varepsilon_f\pm\sqrt{(\varepsilon_k-\varepsilon_f)^2+4|V_k|^2})$$

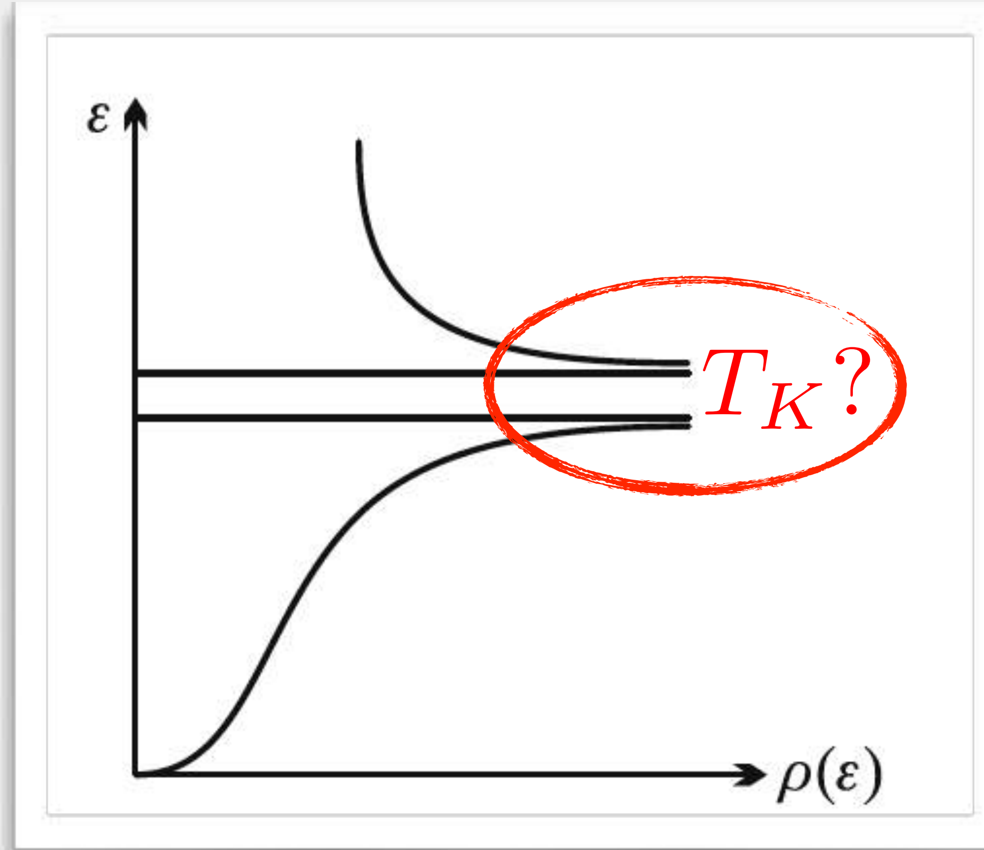
$$H = \sum_{k,\sigma} \varepsilon_k c^{\dagger}_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \varepsilon_f f^{\dagger}_{k,\sigma} f_{k,\sigma} + \sum_{k,\sigma} (V_k c^{\dagger}_{k,\sigma} f_{k,\sigma} + V^*_k f^{\dagger}_{k,\sigma} c_{k,\sigma})$$

$$E^{\pm}_k = \frac{1}{2}(\varepsilon_k + \varepsilon_f \pm \sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4|V_k|^2})$$









The relevant question is how interactions renormalize these bands and, in particular, how to obtain a minigap of the order of Tk characteristic of heavy fermion "Kondo insulators"

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \varepsilon_f f^\dagger_{k,\sigma} f_{k,\sigma} + \sum_{k,\sigma} (V_k c^\dagger_{k,\sigma} f_{k,\sigma} + V^*_k f^\dagger_{k,\sigma} c_{k,\sigma})$$

$$\xrightarrow{?}$$

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \tilde{\varepsilon}_f f^\dagger_{k,\sigma} f_{k,\sigma} + \sum_{k,\sigma} (\tilde{V}_k c^\dagger_{k,\sigma} f_{k,\sigma} + \tilde{V}^*_k f^\dagger_{k,\sigma} c_{k,\sigma})$$

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Doniach's Kondo lattice

Simpler than Anderson, Doniach just considered spins on a lattice

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \sum_j \sum_{\alpha\beta} \vec{S}_j . c^\dagger_{k\alpha} \vec{\sigma}_{\alpha\beta} c_{k'\beta} e^{i(k'-k).R_j}$$

Most local moments develop an antiferromagnetic order at low temperatures. A magnetic moment at a given location induces a wave of Friedel oscillations in the electron spin density (RKKY interaction, Mª José Calderón's lectures)

$$\langle \vec{\sigma}(x) \rangle = -J\chi(x - x_0) \langle \vec{S}(x_0) \rangle$$

$$\chi(x - x_0) = 2 \sum_{k,k'} \left(\frac{f(\varepsilon_k) - f(\varepsilon_{k'})}{\varepsilon_{k'} - \varepsilon_k} \right) e^{i(k-k')x}$$

Non-local susceptibility

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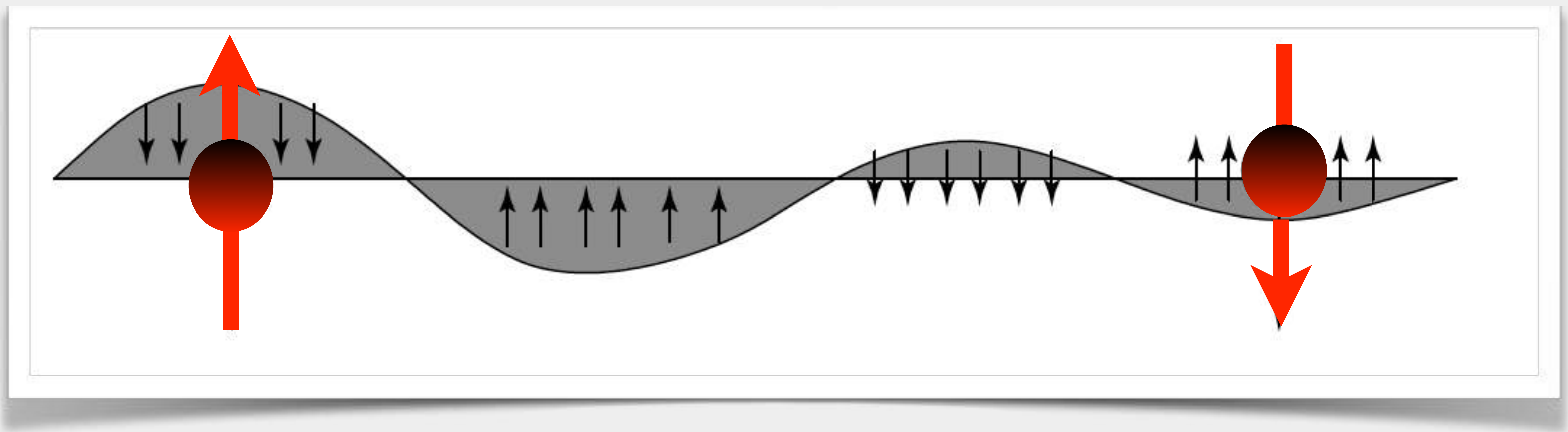
$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \sum_j \sum_{\alpha\beta} \vec{S}_j . c^\dagger_{k\alpha} \vec{\sigma}_{\alpha\beta} c_{k'\beta} e^{i(k'-k).R_j}$$

Doniach's Kondo lattice

$$\langle \vec{\sigma}(x) \rangle = -J\chi(x - x_0) \langle \vec{S}(x_0) \rangle$$

$$\langle \vec{\sigma}(r) \rangle \sim -J\rho \frac{cos 2k_F r}{|k_F r|^3}$$



$$H_{RKKY} = -\frac{J^2}{2} \sum_{x,x_0} \chi(x - x_0) \vec{S}(x) . \vec{S}(x_0)$$

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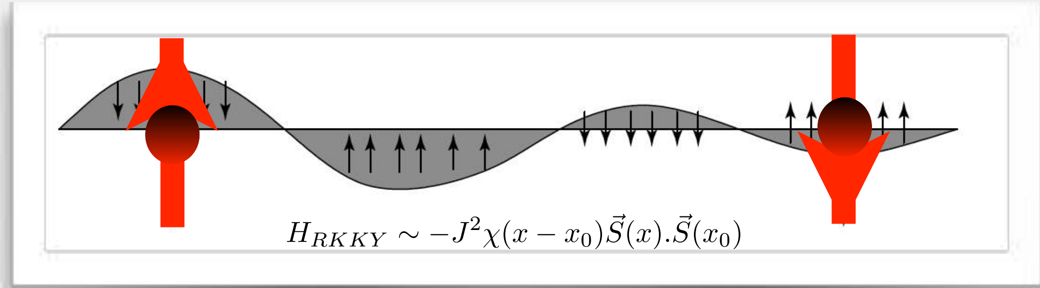
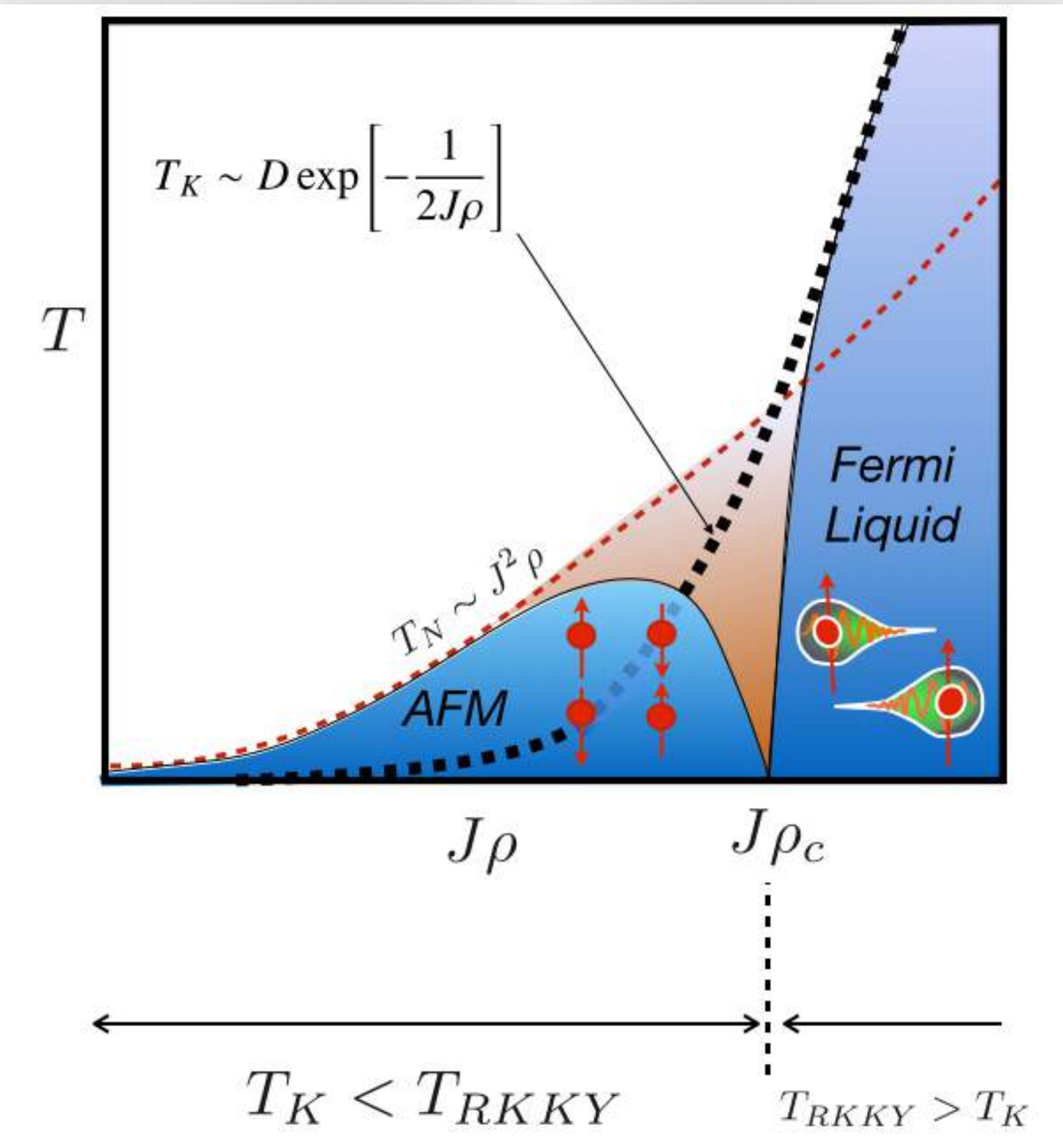
Doniach's Kondo lattice



Competition of two energy scales



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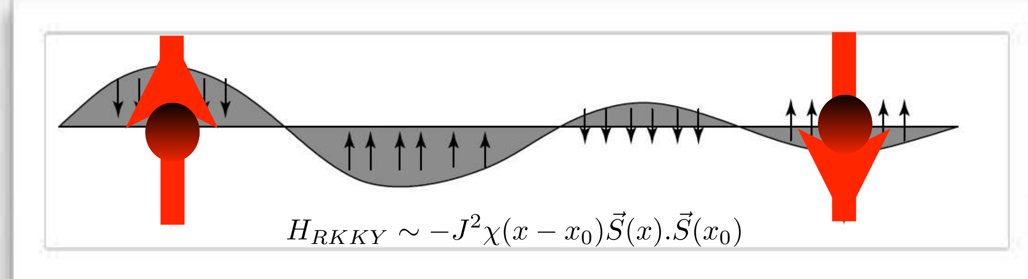
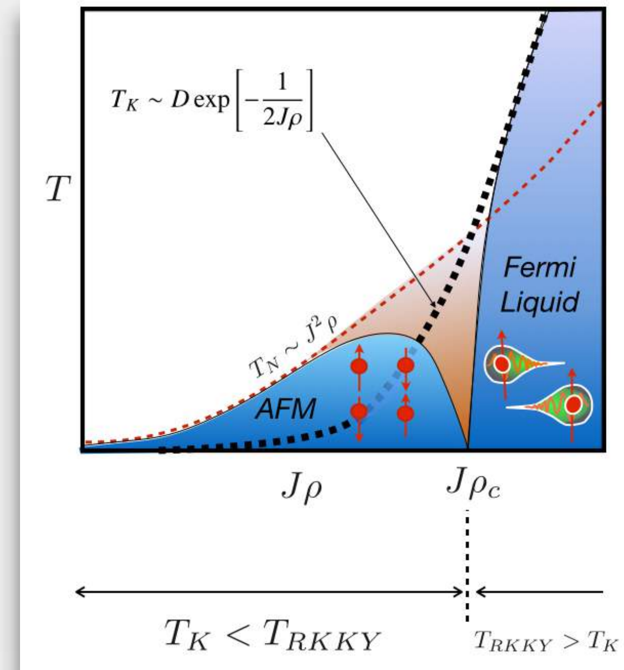
Doniach's Kondo lattice





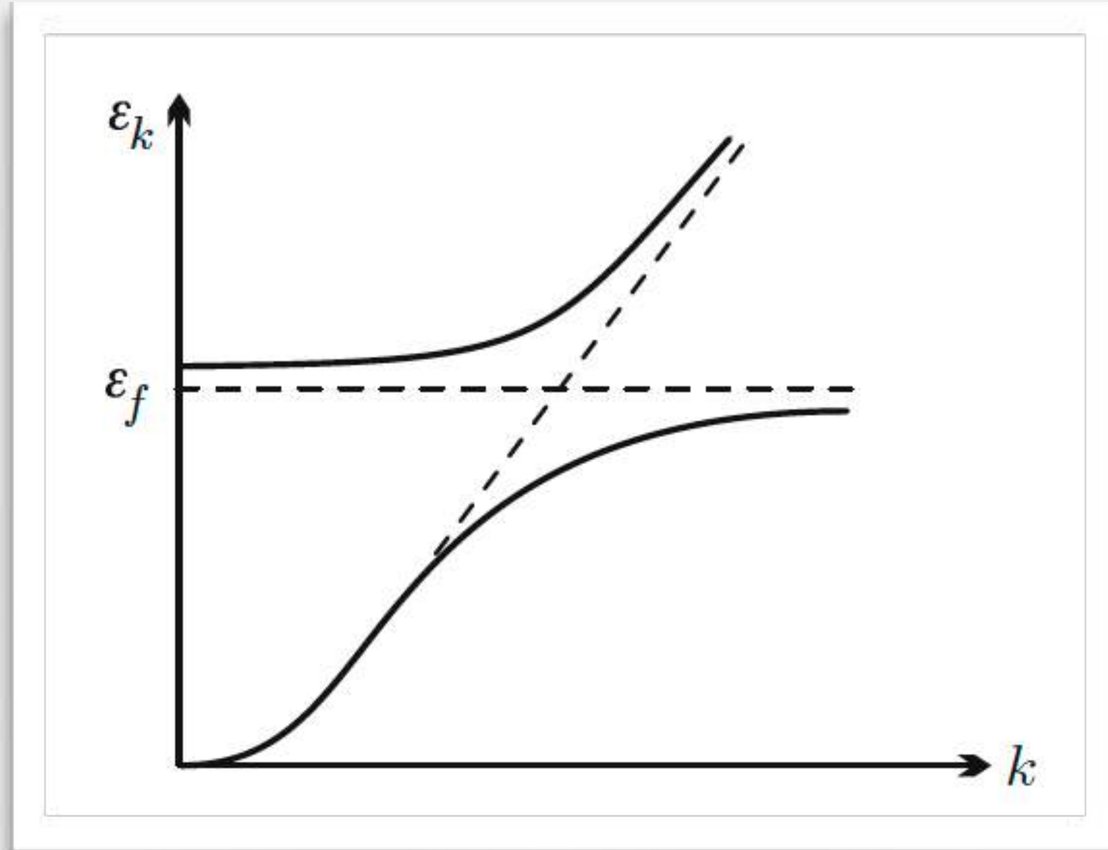
Competition of two energy scales

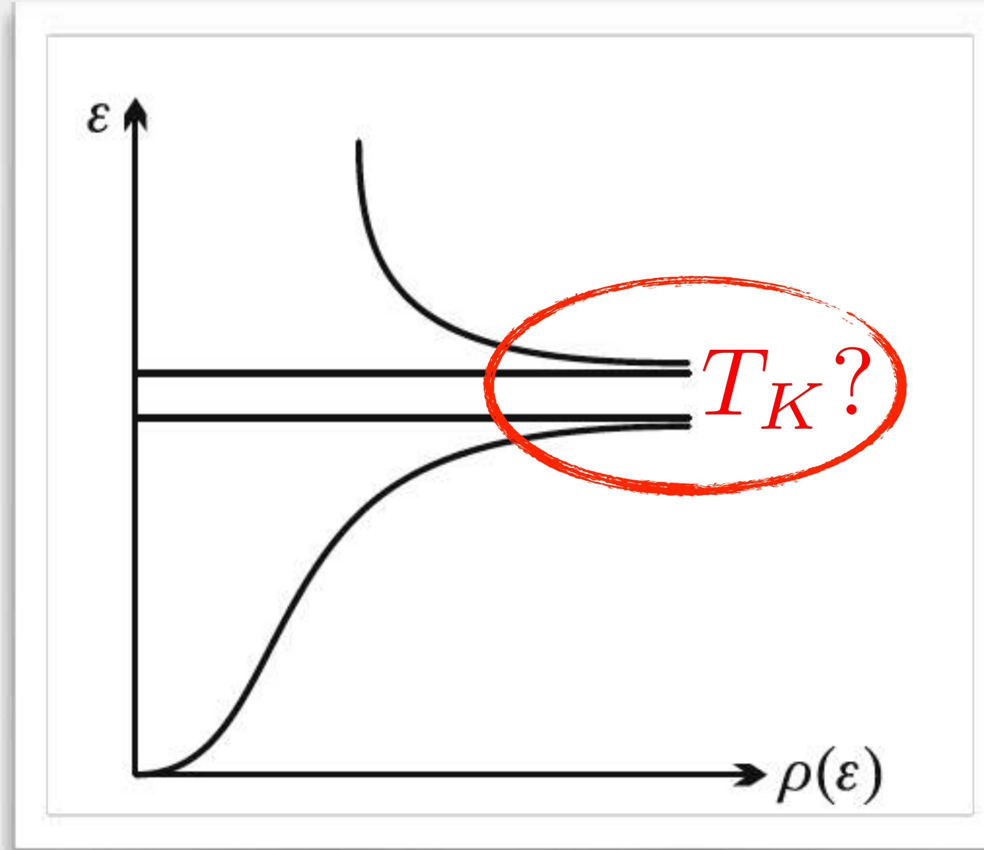
Minimal realization where this competition already appears: the two-impurity Kondo problem, the ground state changes from Kondo singlet to AF singlet when

$$\frac{J}{T_K} \sim 2$$

B. A. Jones, C. M. Varma, and J. W. Wilkins, Low-temperature properties of the two-impurity Kondo hamiltonian. Phys. Rev. Lett. 61, 125–128 (1988).

How to treat lattices beyond this phenomenological picture? A powerful technique to capture the strong coupling limit is the large N approach





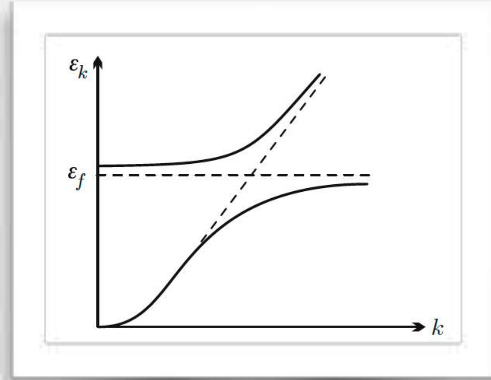
The relevant question is how interactions renormalize these bands and, in particular, how to obtain a minigap of the order of Tk characteristic of heavy fermion "Kondo insulators"

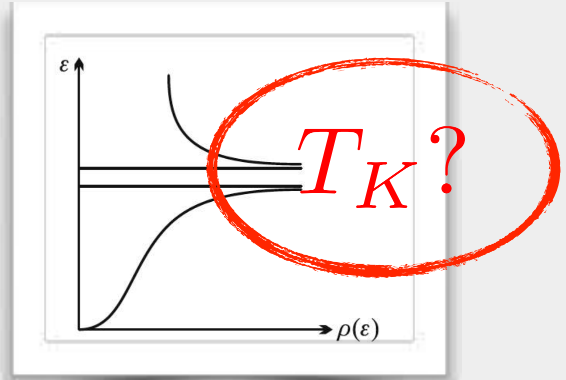
$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \varepsilon_f f^\dagger_{k,\sigma} f_{k,\sigma} + \sum_{k,\sigma} (V_k c^\dagger_{k,\sigma} f_{k,\sigma} + V^*_k f^\dagger_{k,\sigma} c_{k,\sigma})$$

$$\xrightarrow{?}$$

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \tilde{\varepsilon}_f f^\dagger_{k,\sigma} f_{k,\sigma} + \sum_{k,\sigma} (\tilde{V}_k c^\dagger_{k,\sigma} f_{k,\sigma} + \tilde{V}^*_k f^\dagger_{k,\sigma} c_{k,\sigma})$$

CSIC





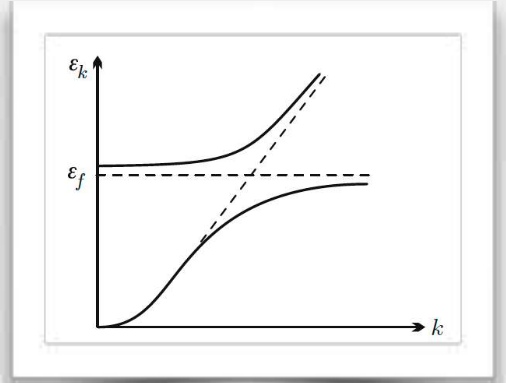
$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{i,\sigma} \varepsilon_f f^\dagger_{i,\sigma} f_{i,\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} +$$

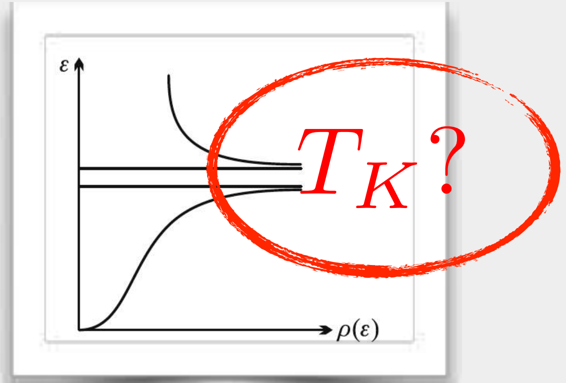
$$\sum_{i,k,\sigma} (V_k e^{-ik.R_i} c^\dagger_{k,\sigma} f_{i,\sigma} + V^*_k e^{ik.R_i} f^\dagger_{i,\sigma} c_{k,\sigma})$$

Narrow f-bands, such as Cerium, the ratio U to the band width is extremely large:

$$U \to \infty$$

Double occupancy of the orbitals becomes <u>forbidden</u>





$$U \to \infty$$

Double occupancy of the orbitals becomes <u>forbidden</u>

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{\sigma} \varepsilon_f |1,\sigma\rangle\langle 1,\sigma| + \sum_{k,\sigma} V_k c^\dagger_{k,\sigma} |0,0\rangle\langle 1,\sigma| + V^*_k |1,\sigma\rangle\langle 0,0| c_{k,\sigma}$$

On each site

$$X_{pq} = |p\rangle\langle q|$$

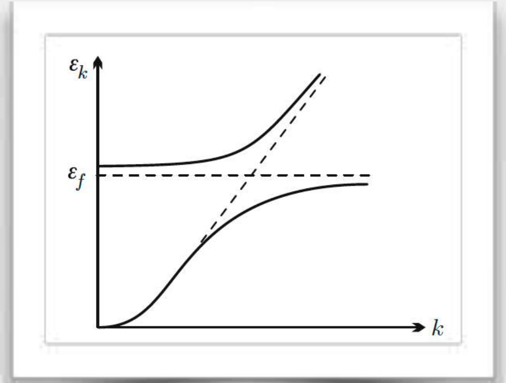
are Hubbard operators that restrict the Hilbert space to the desired physical sector, such constraint is just given by the completeness relation

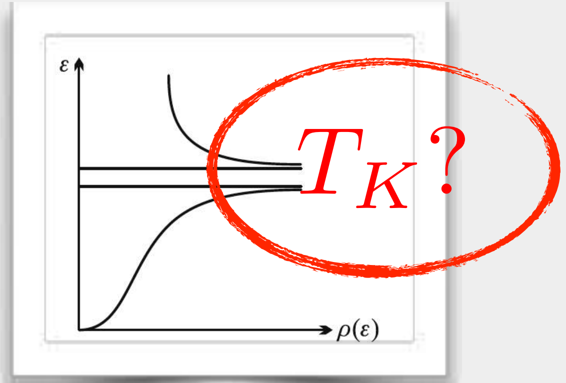
$$\sum_q X_{qq} = |q\rangle\langle q| = 1$$

Note: these many-body operators do not follow standard commutation/anticommutation rules

$$|q\rangle\langle p|p'\rangle\langle q'| = \delta_{p,p'} |q\rangle\langle q'|$$

Similar to spin operators, Wicks theorem is not valid and standard perturbation theory <u>cannot</u> be applied.





$$U \to \infty$$

Double occupancy of the orbitals becomes forbidden

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{\sigma} \varepsilon_f |1,\sigma\rangle\langle 1,\sigma| + \sum_{k,\sigma} V_k c^\dagger_{k,\sigma} |0,0\rangle\langle 1,\sigma| + V^*_k |1,\sigma\rangle\langle 0,0| c_{k,\sigma}$$

On each site

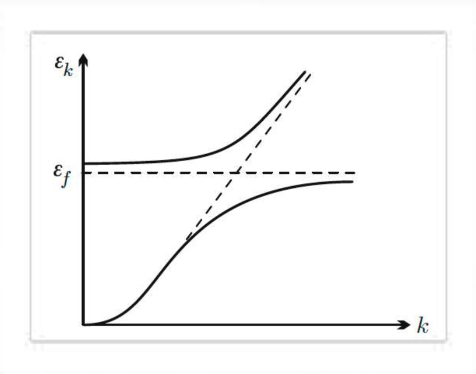
$$f_\sigma \to |0,0\rangle\langle 1,\sigma| \qquad f^\dagger_\sigma \to |1,\sigma\rangle\langle 0,0|$$

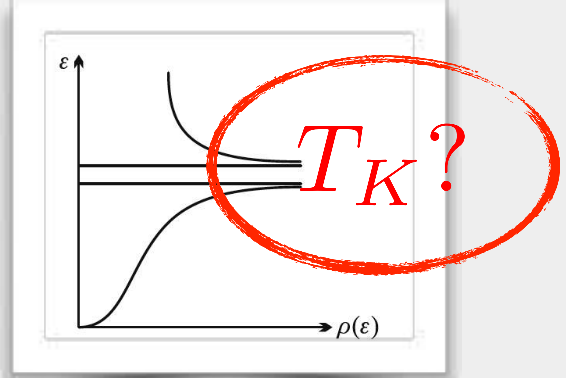
$$X_{pq} = |p\rangle\langle q|$$

$$\sum_q X_{qq} = |q\rangle\langle q| = 1 \longrightarrow \sum_\sigma f^\dagger_\sigma f_\sigma + |0,0\rangle\langle 0,0| = 1$$

Trick: replace physical fermion by slave boson and fermion (exact). Physically these degrees of freedom represent charge fluctuations and spin fluctuations, respectively.

$$f^\dagger_\sigma \to d^\dagger_\sigma b$$





$$U \to \infty$$

Double occupancy of the orbitals becomes forbidden

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_\sigma \varepsilon_f |1,\sigma\rangle\langle 1,\sigma| + \sum_{k,\sigma} V_k c^\dagger_{k,\sigma} |0,0\rangle\langle 1,\sigma| + V_k^* |1,\sigma\rangle\langle 0,0| c_{k,\sigma}$$

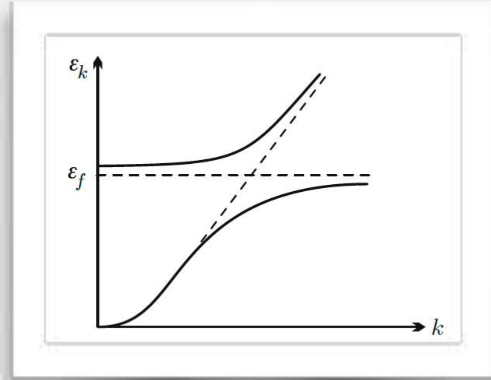
$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_\sigma \varepsilon_f d^\dagger_\sigma d_\sigma + \sum_{k,\sigma} V_k c^\dagger_{k,\sigma} d_\sigma b^\dagger + V_k^* d^\dagger_\sigma c_{k,\sigma} b$$

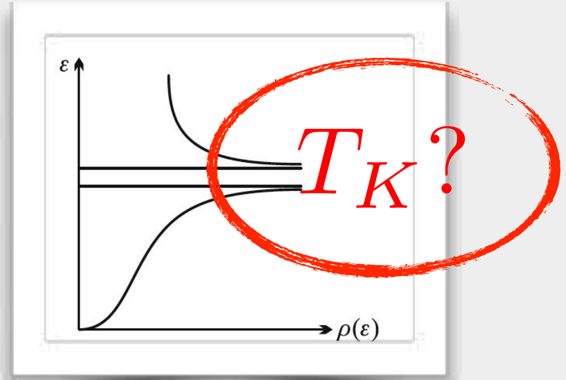
Three operator vertex containing fermions and bosons!

Provided that we work with the constraint

$$\sum_\sigma d^\dagger_\sigma d_\sigma + b^\dagger b = 1$$

Read &Newns, J. Phys. C, 16, 3273 (1983)
Coleman, Phys. Rev B, 29, 3035 (1984)





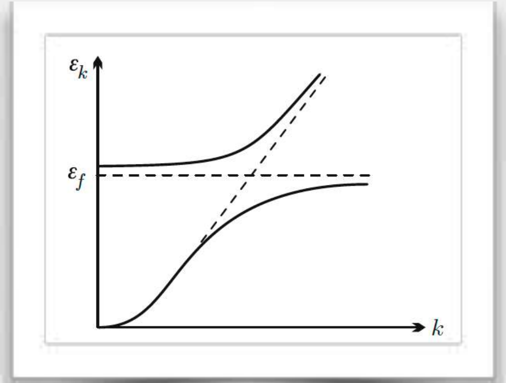
$$U \rightarrow \infty$$

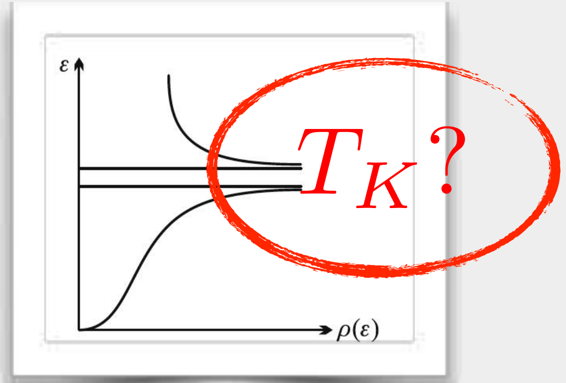
Double occupancy of the orbitals becomes forbidden

Work with generalized Hamiltonian, includes Lagrange multiplier to take care of constraint

$$H(\lambda) = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{\sigma} \varepsilon_f d^\dagger_\sigma d_\sigma + \sum_{k,\sigma} V_k c^\dagger_{k,\sigma} d_\sigma b^\dagger + V^*_k d^\dagger_\sigma c_{k,\sigma} b + \lambda(b^\dagger b + \sum_\sigma d^\dagger_\sigma d_\sigma - 1)$$

Constraint





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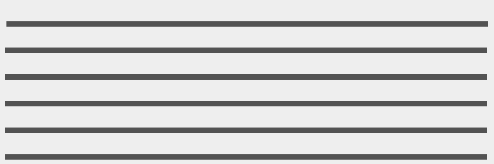
Constraint

$$\sum_{\sigma=1}^{N}$$

Remember: f local moments
have large degeneracies



Low lying magnetic multiplet

$$N = 2j + 1$$

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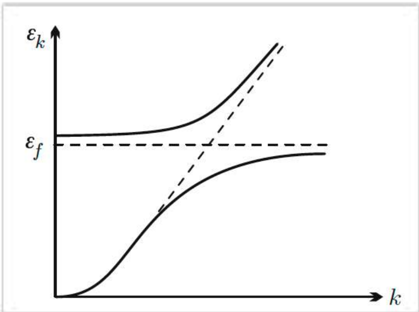

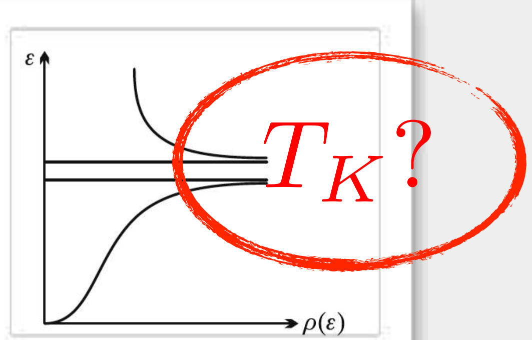

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- One can perform controlled $\frac{1}{N}$ expansions

- The "mean field" limit $N \to \infty$ gives the strong coupling limit we seek!

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Large N

$$H_I(j) = \frac{J}{N} S_{\alpha\beta}(j).c^{\dagger}_{j\alpha} c_{j\beta} = -\frac{J}{N}(c^{\dagger}_{j\beta} f_{j\beta})(f^{\dagger}_{j\alpha} c_{j\alpha})$$

This kind of interaction can be factorized using Hubbard-Stratonovich

$$-gA^{\dagger}A \rightarrow A^{\dagger}V + \bar{V}A + \frac{\bar{V}V}{g}$$

$$H_I(j) \rightarrow \bar{V}_j(c^{\dagger}_{j\beta} f_{j\beta}) + (f^{\dagger}_{j\alpha} c_{j\alpha})V_j + N\frac{\bar{V}_j V_j}{J}$$

Exact provided that the auxiliary V are treated as quantum fluctuating fields. As we have seen, these fields <u>have a physical meaning</u> in the context of the Anderson model ("slave bosons" that govern valence fluctuations).

Large N

$$H_I(j) \rightarrow \bar{V}_j (c^\dagger_{j\beta} f_{j\beta}) + (f^\dagger_{j\alpha} c_{j\alpha}) V_j + N \frac{\bar{V}_j V_j}{J}$$

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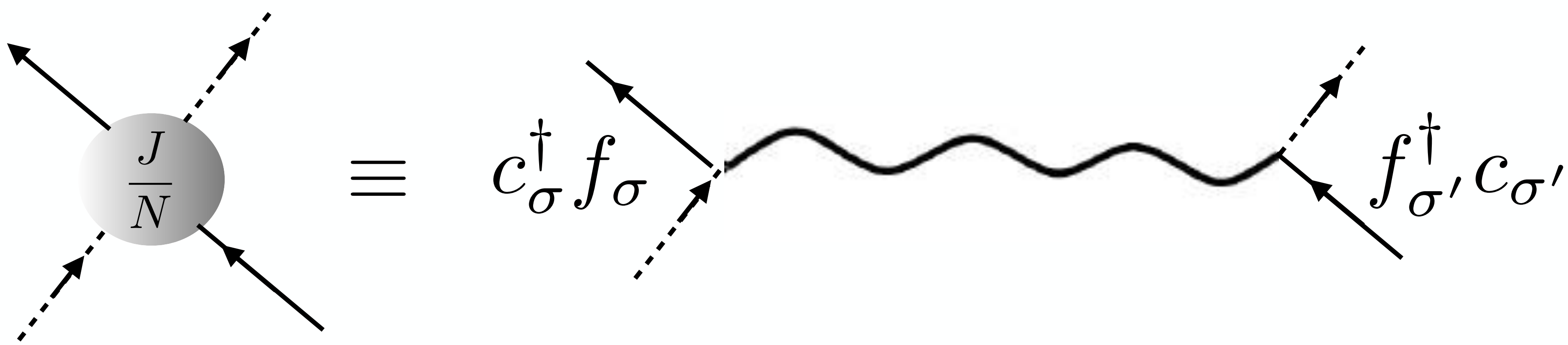
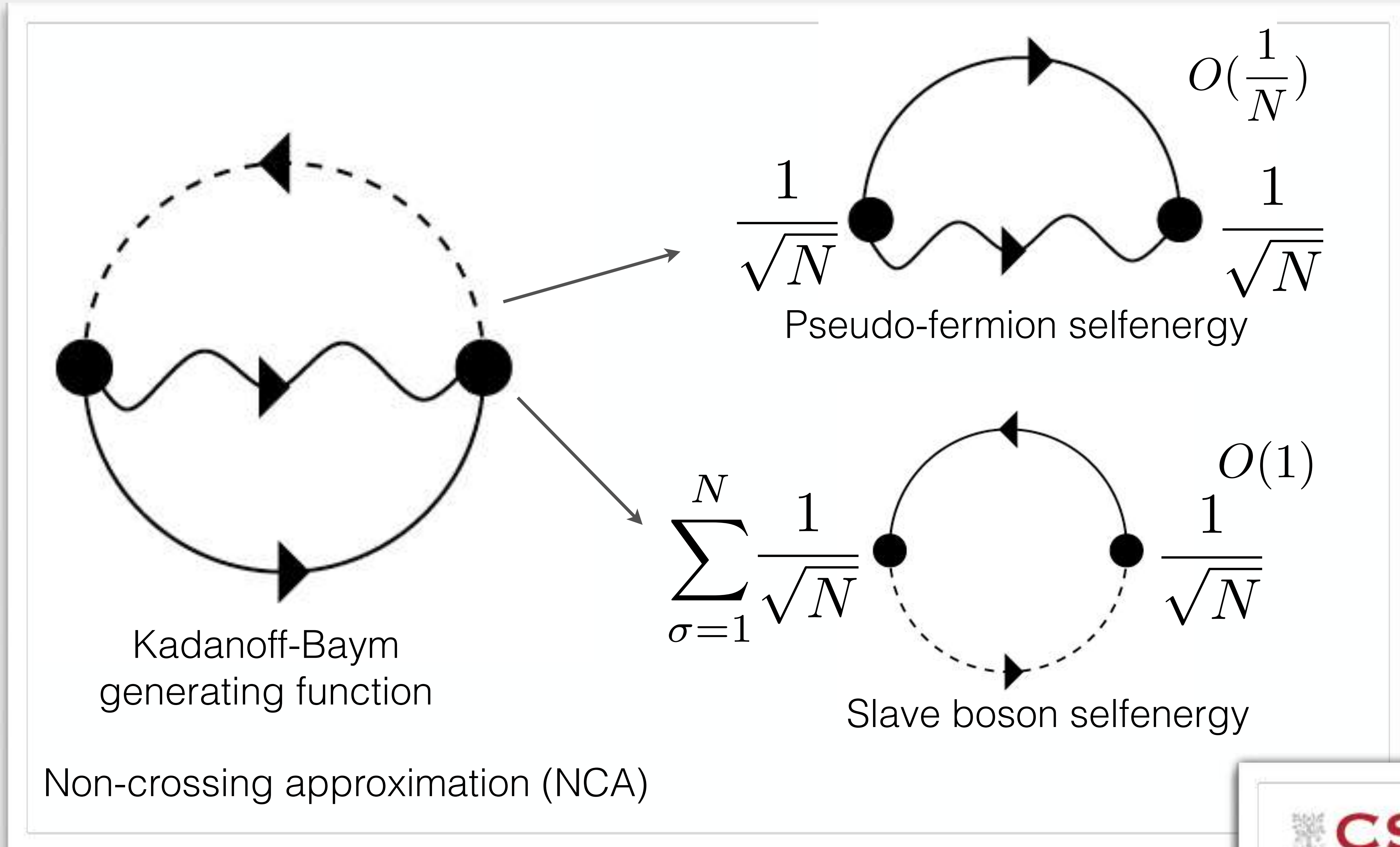


$$-\frac{J}{N}(c^\dagger_\sigma f_\sigma)(f^\dagger_{\sigma'} c_{\sigma'})$$

Large N

- Very powerful method as it allows systematic expansion in $\frac{1}{N}$



Large N

- Very powerful method as it allows systematic expansion in $\frac{1}{N}$

- Non-perturbative self-consistent expansion.

- It can be generalized to non-equilibrium using Keldysh Green's functions techniques. As we will see, very useful for Kondo transport in nanostructures

  - David C. Langreth and Peter Nordlander, Phys. Rev. B, 43, 2541 (1991).
  - Ned Wingreen and Yigal Meir, Phys. Rev. B 49, 11040 (1994)
  - Ramón Aguado and David C. Langreth, Phys. Rev. B 67, 245307 (2003)

$$U \to \infty$$

Double occupancy of the orbitals becomes forbidden

$$H(\lambda) = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_\sigma \varepsilon_f d^\dagger_\sigma d_\sigma + \frac{V_0}{\sqrt{N}} \sum_{k,\sigma} (c^\dagger_{k,\sigma} d_\sigma b^\dagger + d^\dagger_\sigma c_{k,\sigma} b) + \lambda(b^\dagger b + \sum_\sigma d^\dagger_\sigma d_\sigma - 1)$$

Mean field

$$H(\lambda) = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_\sigma \varepsilon_f d^\dagger_\sigma d_\sigma + \frac{V_0 \langle b \rangle}{\sqrt{N}} \sum_{k,\sigma} (c^\dagger_{k,\sigma} d_\sigma + d^\dagger_\sigma c_{k,\sigma}) + \lambda(\langle b \rangle^2 + \sum_\sigma d^\dagger_\sigma d_\sigma - 1)$$

Renormalized parameters

$$\tilde{V} = \frac{V_0 \langle b \rangle}{\sqrt{N}} = V_0 \tilde{b} \qquad \tilde{\varepsilon}_f = \varepsilon_f + \lambda$$

$U \to \infty$

Double occupancy of the orbitals becomes forbidden

$$H(\lambda) = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_\sigma \varepsilon_f d^\dagger_\sigma d_\sigma + \frac{V_0 \langle b \rangle}{\sqrt{N}} \sum_{k,\sigma} (c^\dagger_{k,\sigma} d_\sigma + d^\dagger_\sigma c_{k,\sigma}) + \lambda(\langle b \rangle^2 + \sum_\sigma d^\dagger_\sigma d_\sigma - 1)$$

Effective non-interacting resonant level model with renormalized parameters!!

$$\tilde{V} = \frac{V_0 \langle b \rangle}{\sqrt{N}} = V_0 \tilde{b} \qquad \tilde{\varepsilon}_f = \varepsilon_f + \lambda$$

$U \to \infty$

Double occupancy of the orbitals becomes forbidden

$$H(\lambda) = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_\sigma \varepsilon_f d^\dagger_\sigma d_\sigma + \frac{V_0 \langle b \rangle}{\sqrt{N}} \sum_{k,\sigma} (c^\dagger_{k,\sigma} d_\sigma + d^\dagger_\sigma c_{k,\sigma}) + \lambda(\langle b \rangle^2 + \sum_\sigma d^\dagger_\sigma d_\sigma - 1)$$

Solution: solve the selfconsistent set of equations

$$\tilde{b}^2 + \frac{1}{N} \sum_\sigma \langle d^\dagger_\sigma d_\sigma \rangle = \frac{1}{N}$$

$$\frac{\tilde{V}}{N} \sum_{k,\sigma} \langle c^\dagger_{k,\sigma} d_\sigma \rangle + (\tilde{\varepsilon}_f - \varepsilon_f) \tilde{b}^2 = 0$$

$$U \to \infty$$

Double occupancy of the orbitals becomes forbidden

$$\tilde{\Gamma} = \pi \tilde{V}^2 \nu(\varepsilon_F) = \tilde{b}^2 \Gamma$$

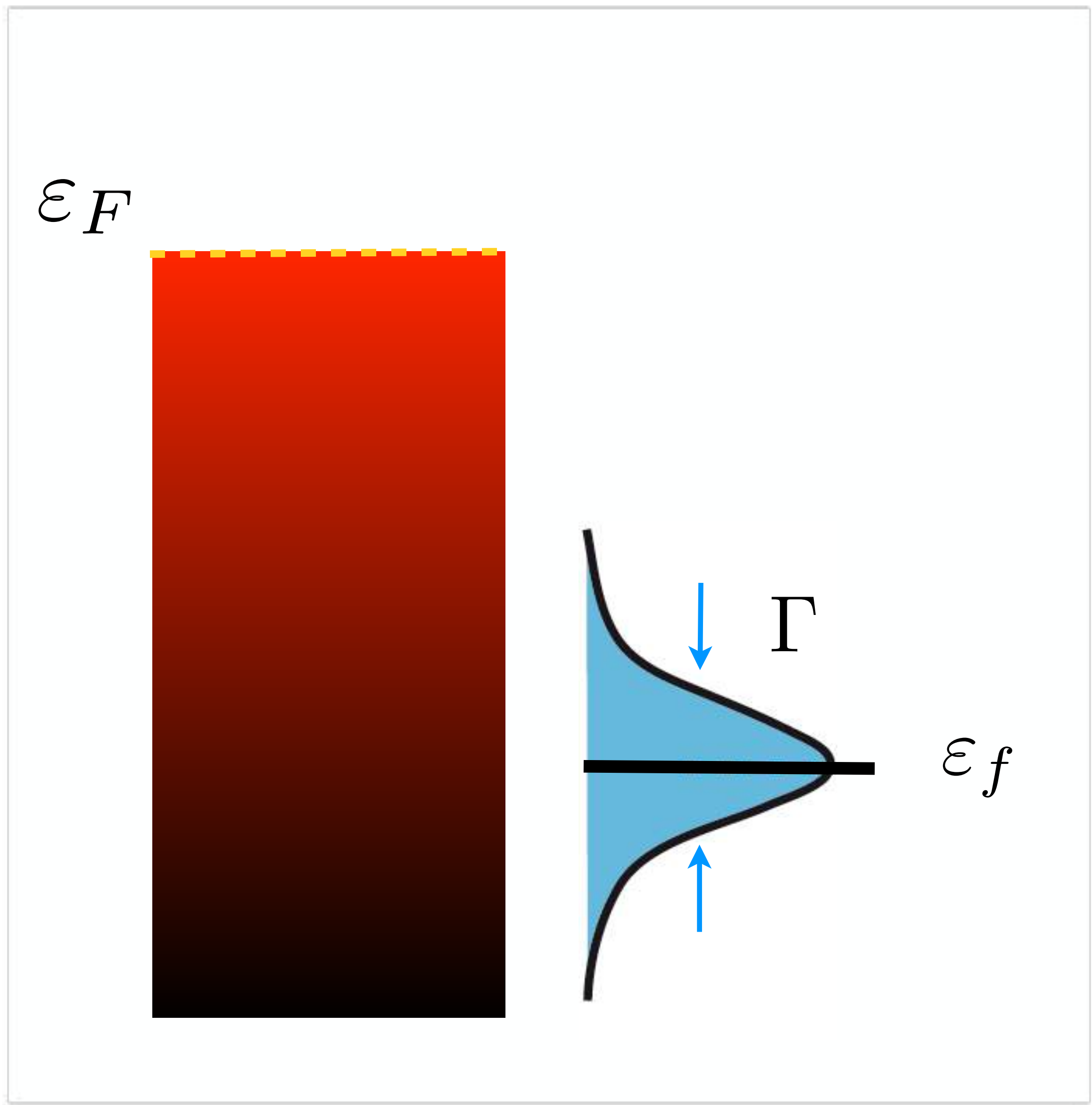
$$\rho(\varepsilon) = \frac{1}{\pi} \frac{\tilde{\Gamma}}{(\varepsilon - \tilde{\varepsilon}_f)^2 + \tilde{\Gamma}^2}$$

$$\sqrt{\tilde{\varepsilon}_f^2 + \tilde{\Gamma}^2} \equiv T_K = D e^{-\frac{\pi |\varepsilon_f|}{N\Gamma}}$$

Exact Kondo temperature!!!!

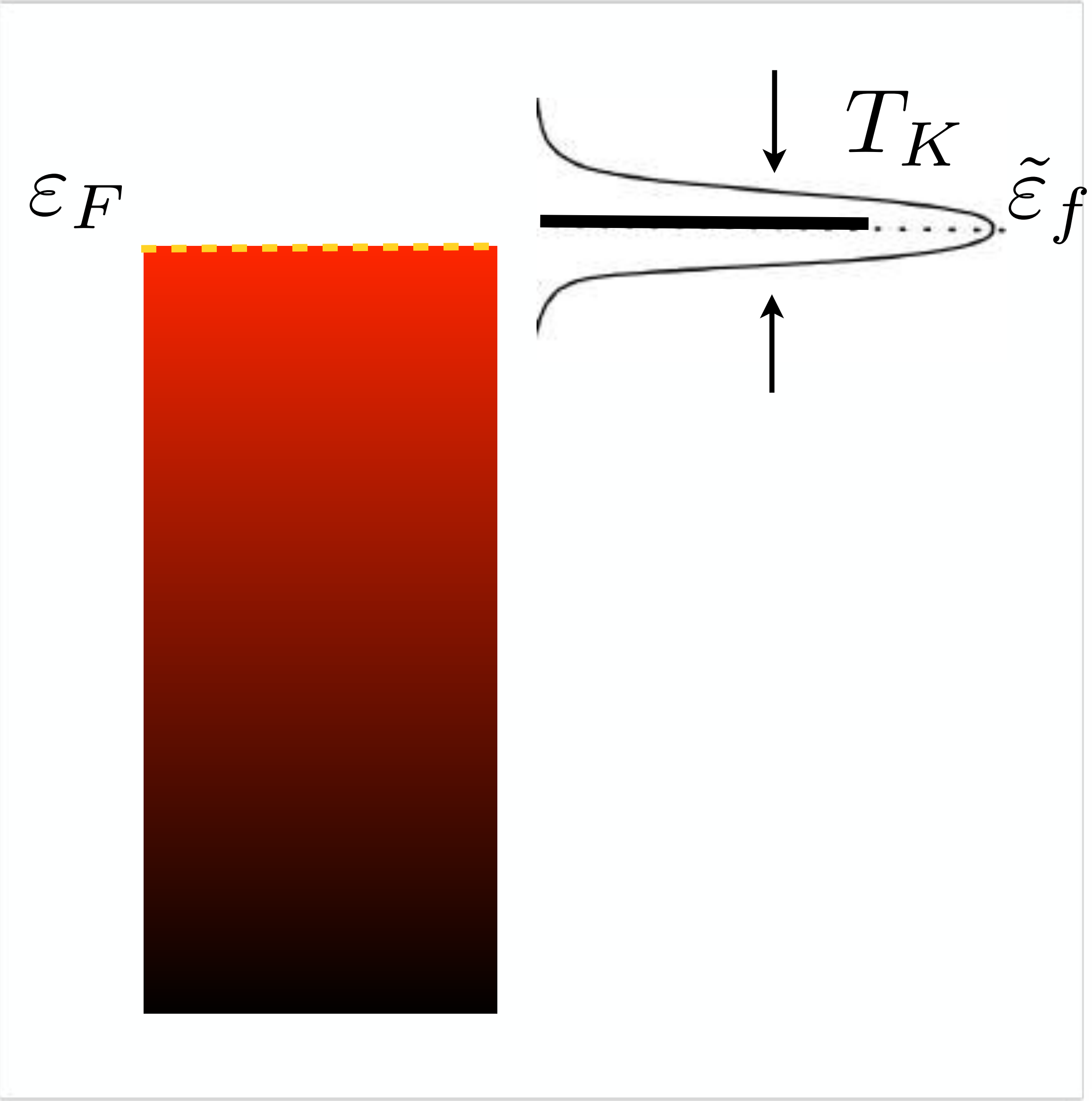
$$U \to \infty$$

Double occupancy of the orbitals becomes forbidden



$$U \to \infty$$

Double occupancy of the orbitals becomes forbidden



$$U \to \infty$$

Double occupancy of the orbitals becomes <u>forbidden</u>

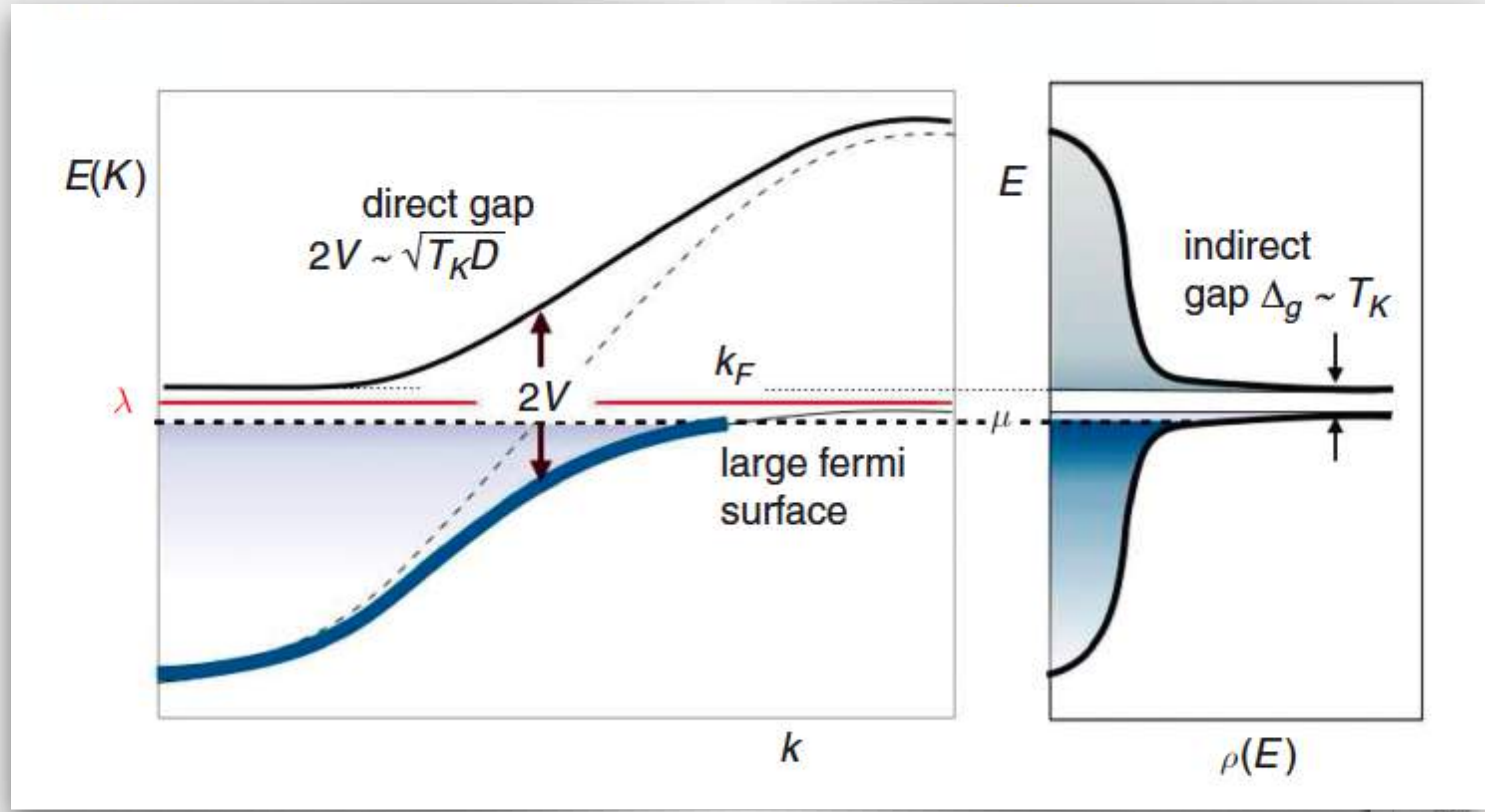
Physical explanation

- For U=0 one would just have a trivial resonant level below the Fermi energy.

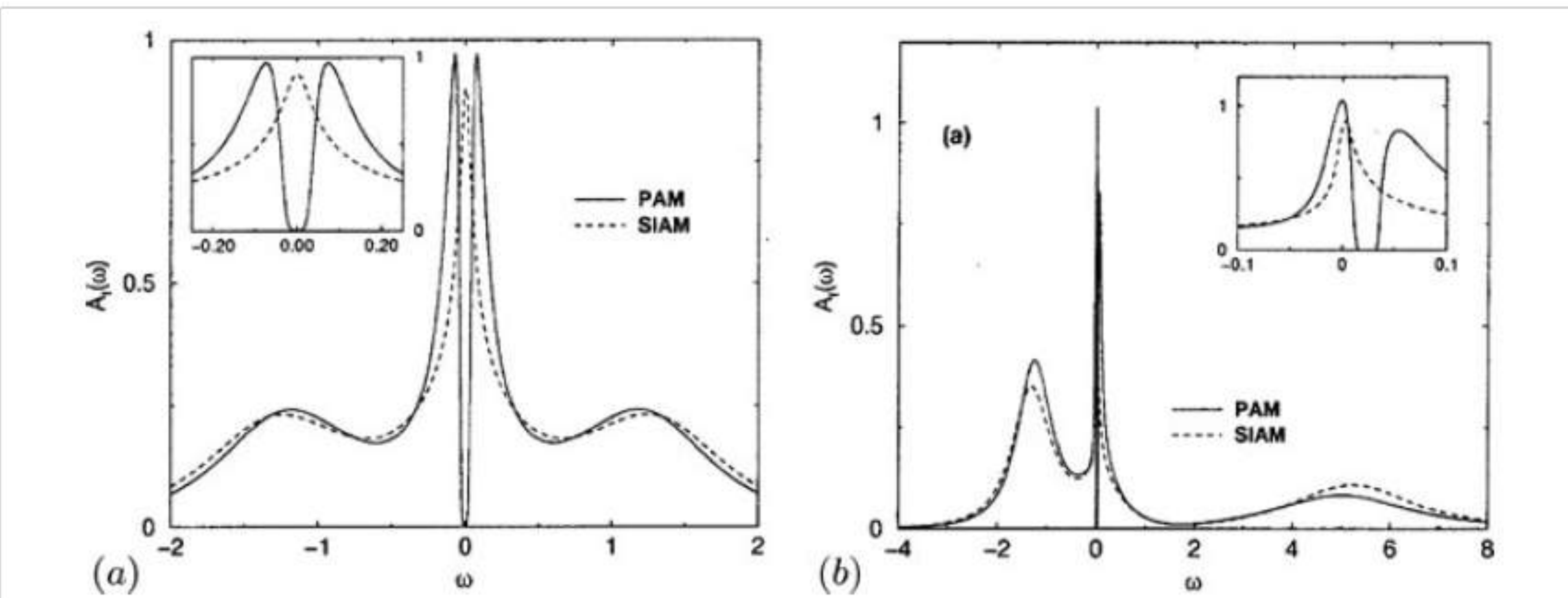
- In the presence of interactions, the constraint forces the resonance to be slightly above the Fermi level while at the same time narrowing it: the hopping amplitude is strongly reduced by the interactions, electrons have to "wait" until the level is empty, this job is taken care of by the slave boson that gives the probability of being empty.

The same method applied to the lattice gives the strong renormalization of the heavy fermion bands

$$E_{k\pm} = \frac{\epsilon_k + \lambda}{2} \pm [(\frac{\epsilon_k - \lambda}{2})^2 + |\tilde{V}|^2]^{\frac{1}{2}}$$



Picture confirmed by Dynamical Mean field calculations of the periodic Anderson model



Th. Pruschke, R. Bulla, and M. Jarrell, Phys. Rev. B 61, 12799 (2000)

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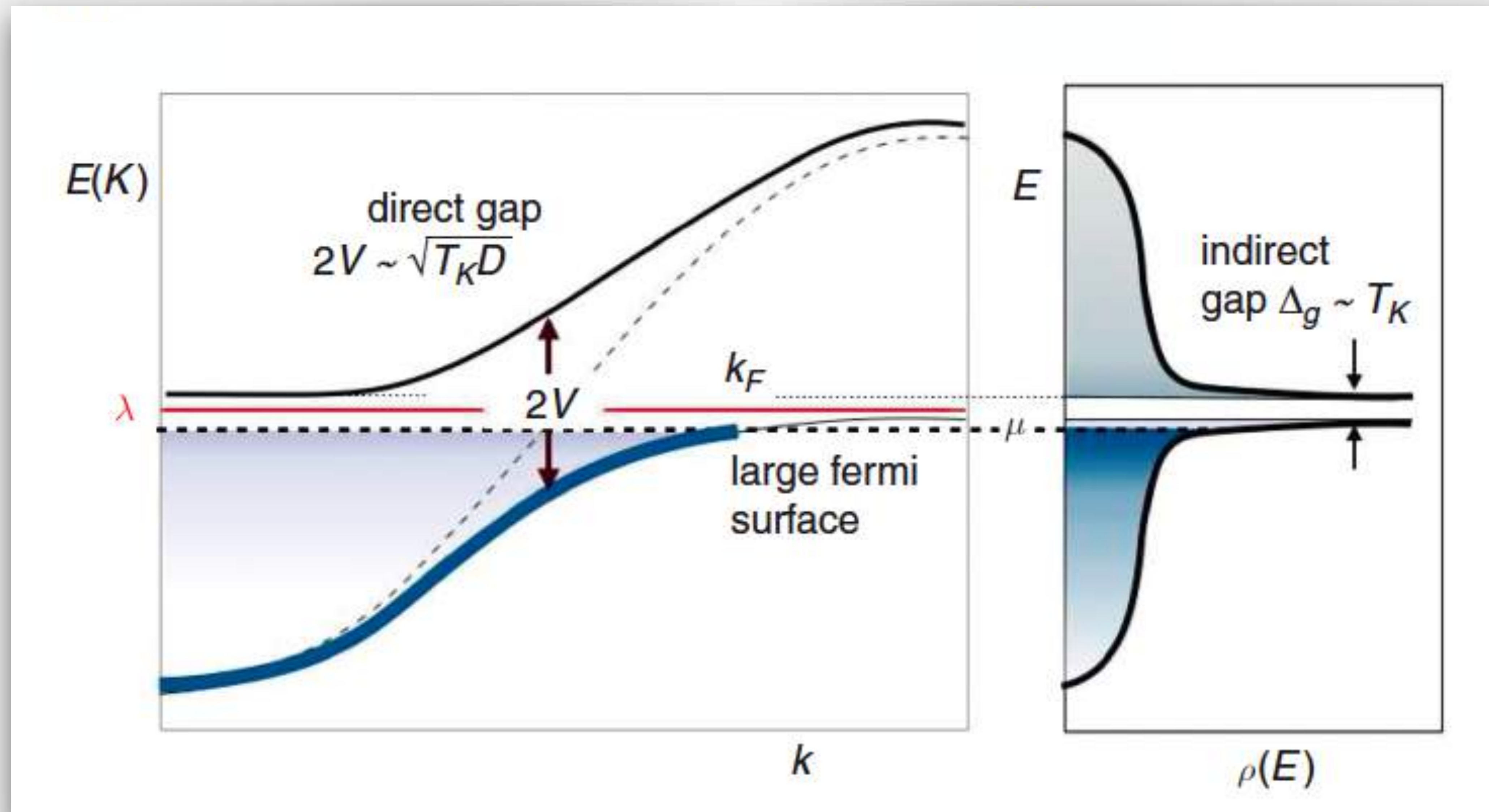
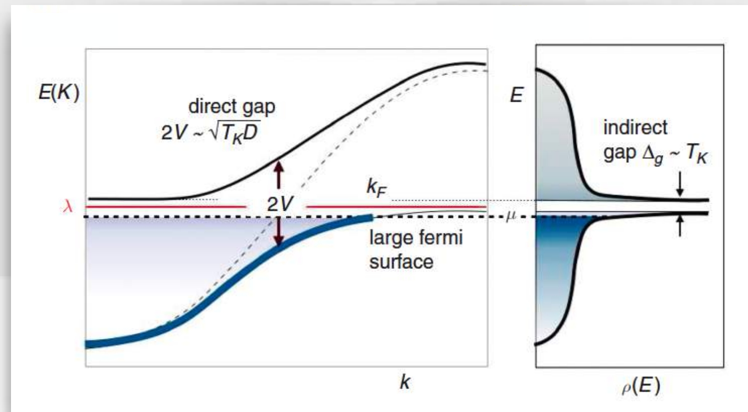
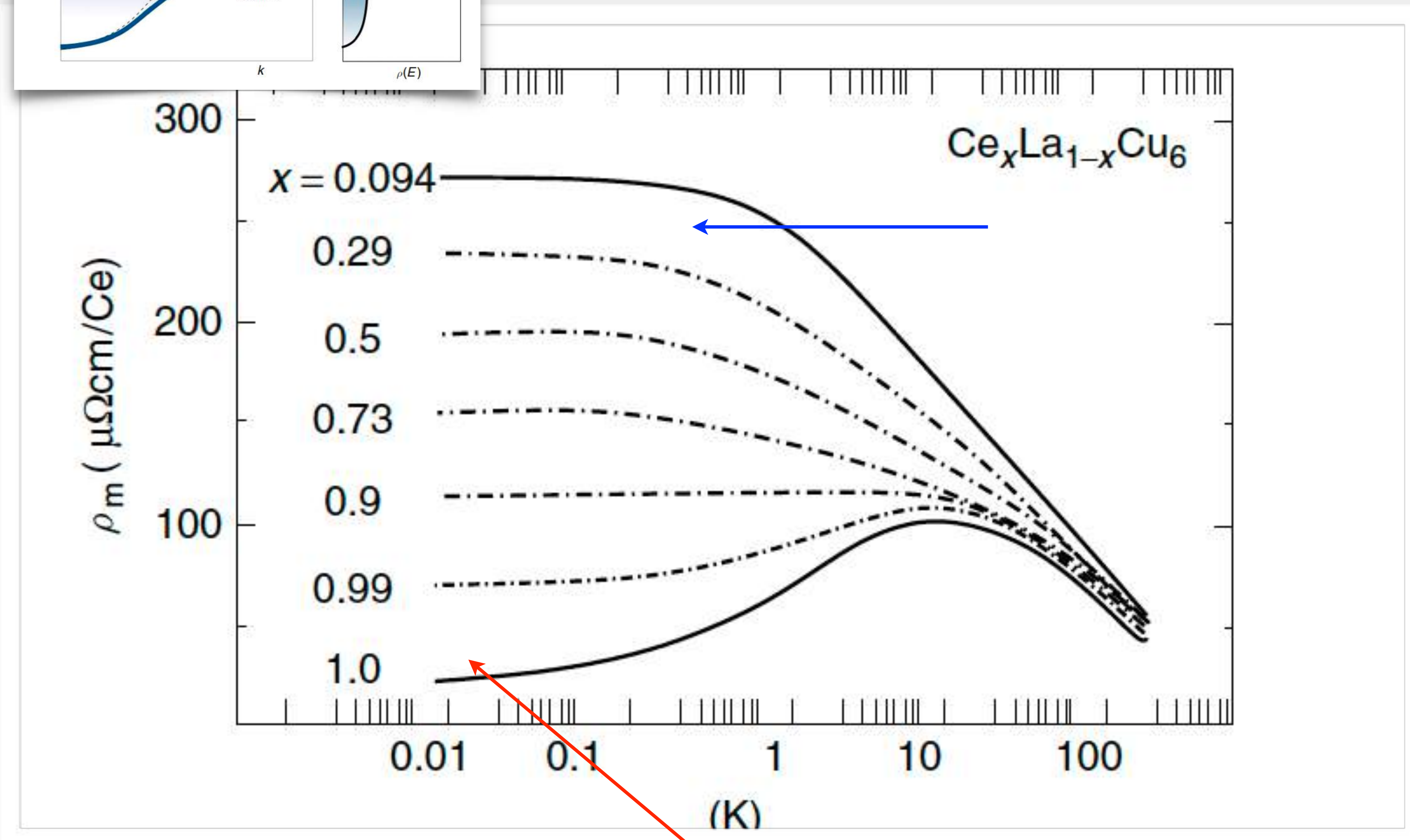
$$E_{k\pm} = \frac{\epsilon_k + \lambda}{2} \pm [(\frac{\epsilon_k - \lambda}{2})^2 + |\tilde{V}|^2]^{\frac{1}{2}}$$



Development of coherence in heavy fermion systems





Development of Coherence: at low enough temperatures, the Kondo increase is quenched by the effective gap

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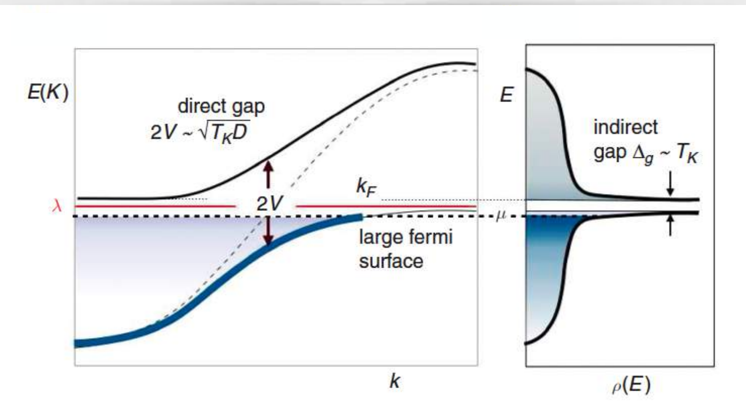


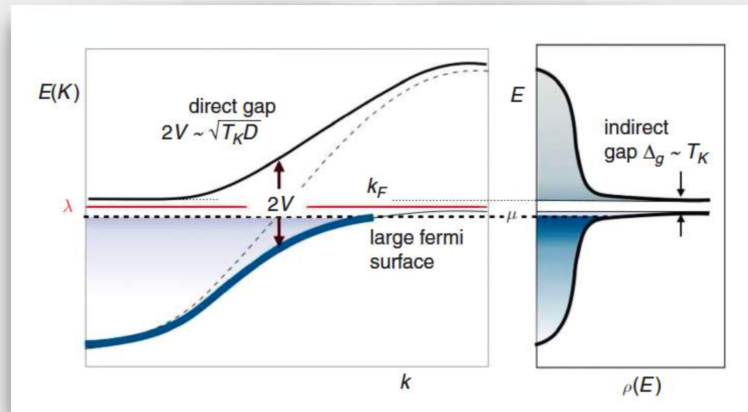
Optical conductivity

According to the f-sum rule, the total integrated optical conductivity is determined by the plasma frequency. In the absence of local moments, this is the total spectral weight inside the Drude peak of the optical conductivity

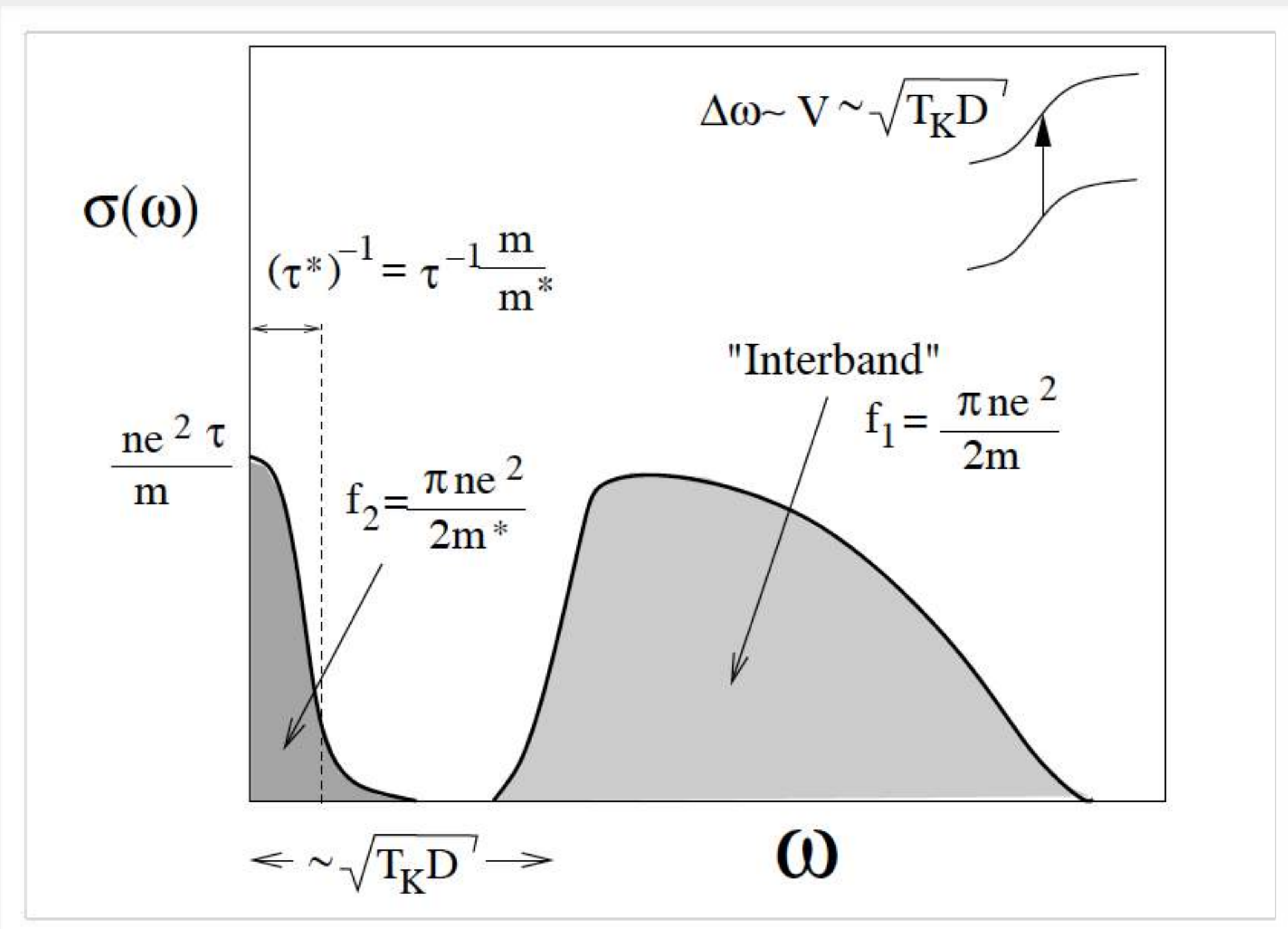
$$\frac{2}{\pi}\int_0^{\infty} d\omega\sigma(\omega) = f_1 = \frac{ne^2}{m}$$

But what happens to the distribution of the spectral weight when the heavy-electron fluid forms? Physically, while we expect this sum rule to be preserved, a new quasiparticle Drude peak will form, corresponding to the heavy-electron Drude peak

$$\frac{2}{\pi}\int_0^{T_K} d\omega\sigma(\omega) = f_2 = \frac{ne^2}{m^*}$$

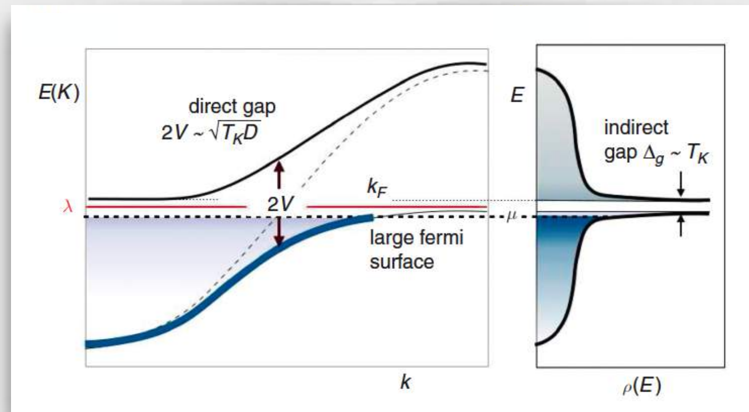


The total spectral weight is divided up into a small "heavy fermion" Drude peak of weight f_2 and a large interband component associated with excitations between lower and upper Kondo bands



$$V \sim \sqrt{T_K D}$$

$$\left(\frac{V}{T_K}\right)^2 \approx \frac{D}{T_K} \sim \frac{m^*}{m}$$



$$\left(\frac{V}{T_K}\right)^2 \approx \frac{D}{T_K} \sim \frac{m^*}{m}$$