Quantum Impurity Solvers for DMFT

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Overview

- **DMFT - A brief recap**
- **Quantum impurity models (QIM)**
- **Numerical approaches to QIM**
  - **Hirsch-Fye quantum Monte Carlo (QMC)**
  - **Numerical renormalization group (NRG)**

DMFT - Brief Recap

- **Motivation: Many interesting unsolved problems in the area of strongly correlated materials (Eg. High T_c cuprates, heavy fermion compounds etc.)**
- **Effective low energy Hamiltonains – simple to write down, hard to solve**
- **Reason: Strong correlations, large couplings...**
- **...**
- **The “simple” Hubbard (“truncated” PPP) model**

$$-t\sum_{ij,\sigma} c^{\dagger}_{i\sigma}c_{j\sigma} - \mu\sum_{i,\sigma} c^{\dagger}_{i\sigma}c_{i\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

on a 2D lattice (is believed to) gives raise to many electronic phases such as the antiferromagnet, superconductor etc.

What are we looking for?

- **We would like to calculate the Green's function**

$$G(\boldsymbol{k}\sigma,\tau)=\langle\mathcal{T}_\tau c_{\boldsymbol{k}\sigma}(\tau)c^\dagger_{\boldsymbol{k}\sigma}(0)\rangle$$

τ **is the imaginary time**

- **We can write this in the frequency domain as**

$$G(\boldsymbol{k}\sigma,\tau)=\frac{1}{\beta}\sum_n G(\boldsymbol{k}\sigma,i\omega_n)e^{-i\omega_n\tau},\omega_n=\frac{(2n+1)\pi}{\beta}$$

- **Analytic continuation of** $G(\boldsymbol{k}\sigma,i\omega_n)$ **from the upper** ω **planes gives us**

$G(\boldsymbol{k}\sigma,i\omega_n)\Longrightarrow$ **Analytical Continuation** $\Longrightarrow G^R(\boldsymbol{k}\sigma,\omega^+)$

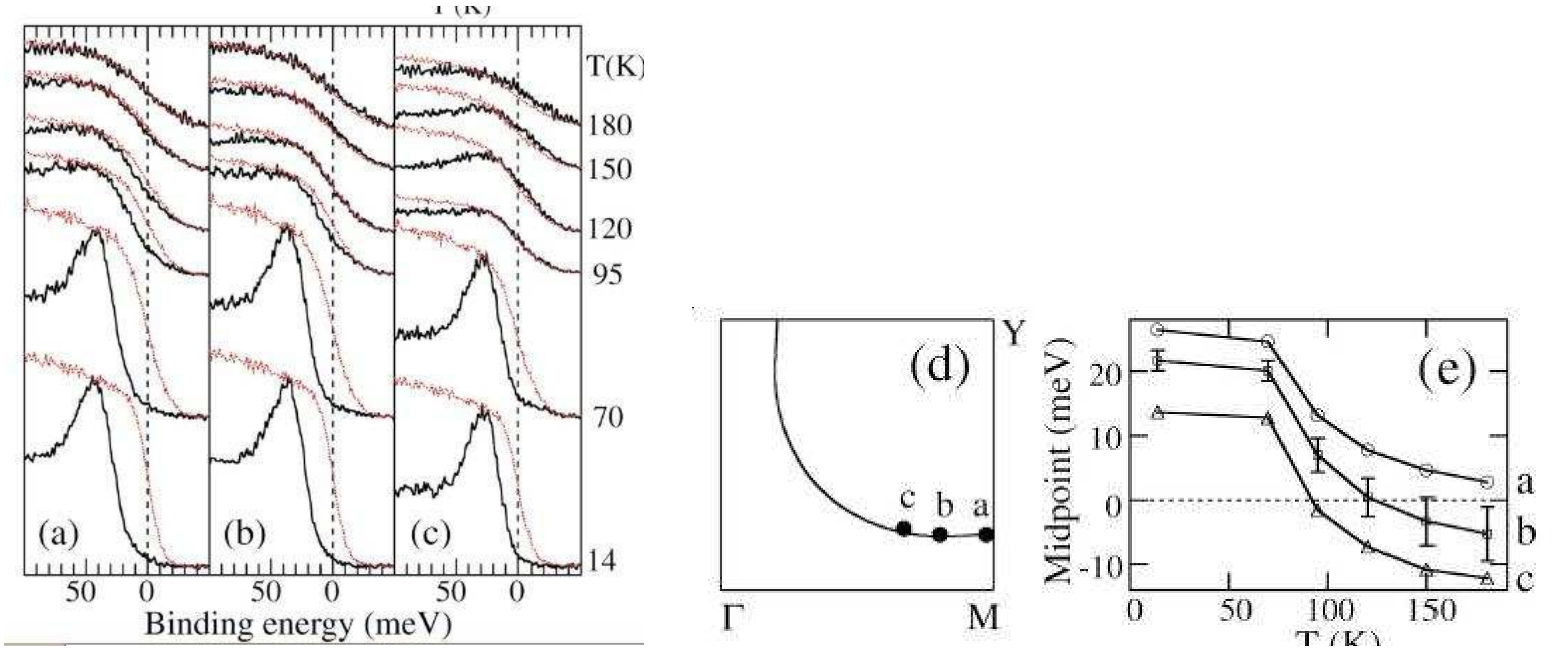
the retarded Green's function

What are we looking for?

- **If we know the retarded Green's function, we can calculate the spectral density**

$$A(\boldsymbol{k}\sigma,\omega) = \frac{1}{\pi}\Im G^R(\boldsymbol{k}\sigma,\omega^+)$$

- **This is an experimentally observable quantity**



VBS **Undoped Bi2212,Damascelli et al. 2003**

Some more elementary ideas

- **The "bare Greens function", G for $U = 0$**

$$G_0(\boldsymbol{k}\sigma, i\omega_n) = \frac{1}{i\omega_n - (\varepsilon(\boldsymbol{k}) - \mu)}$$

$\varepsilon(\boldsymbol{k})$ **– electronic dispersion**

- **The Dyson equation**

$$G^{-1}(\boldsymbol{k}\sigma, i\omega_n) = G_0^{-1}(\boldsymbol{k}\sigma, i\omega_n) - \Sigma(\boldsymbol{k}\sigma, i\omega_n)$$

$\Sigma(\boldsymbol{k}\sigma, i\omega_n)$ **is the "self energy"**

Some more elementary ideas

- **We can define a site Greens function, i – site index**

$$G_{i\sigma}(\tau) = \langle \mathcal{T}_\tau c_{i\sigma}(\tau) c^\dagger_{i\sigma}(0) \rangle$$

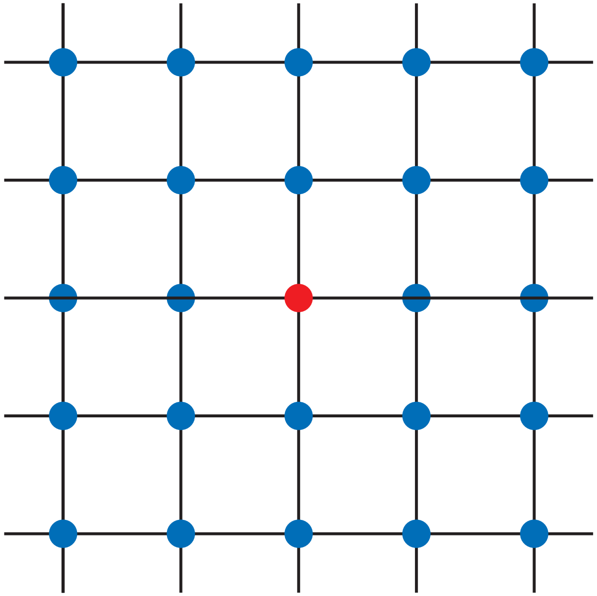
- **In terms of frequency representation, (i - site at the origin)**

$$\begin{aligned} G_{i\sigma}(i\omega_n) &= \frac{1}{N}\sum_{\boldsymbol{k}} G(\boldsymbol{k}\sigma, i\omega_n) \\ &= \frac{1}{N}\sum_{\boldsymbol{k}} \frac{1}{i\omega_n - \varepsilon(\boldsymbol{k}) + \mu - \Sigma(\boldsymbol{k}\sigma, i\omega_n)} \end{aligned}$$

N **- number of sites**

DMFT - Key Ideas

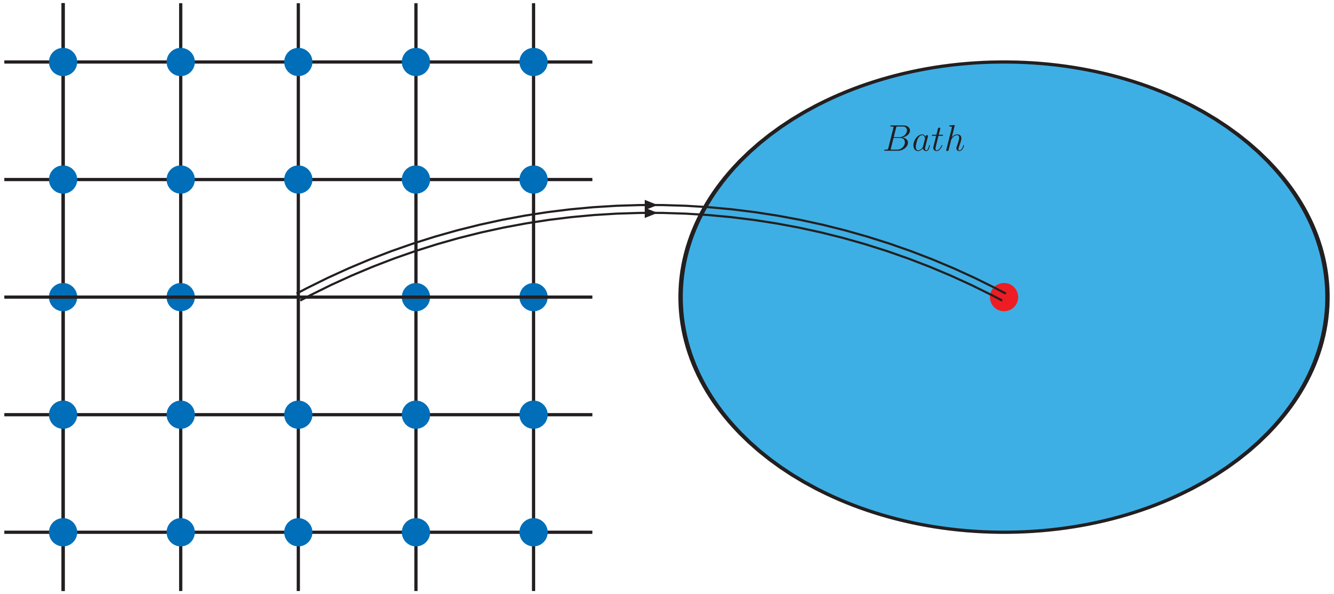
- **Consider the Hubbard model...assume that the system is translationally invariant and focus on** *one site*



- **Question: Can we replace the "other sites" of the lattice by an "effective medium"? If yes, what decides the properties of the medium?**

DMFT - Key Ideas

- Let us replace the "other sites" by a "bath" or "effective medium"



- How do we describe the bath?
- Key point: The bath contains a set of one electron states labeled by α – the *bath by itself is non-interacting!*
- Our site, now an *impurity*, mixes or *hybridizes* with the bath states

DMFT - Key Ideas

- **The bath + impurity, in equations...**

$$\mathcal{H}_A = \underbrace{\sum_\alpha \varepsilon_\alpha b^\dagger_{\alpha\sigma} b_{\alpha\sigma}}_{\textbf{Bath}} + \underbrace{U n_\uparrow n_\downarrow - \mu c^\dagger_\sigma c_\sigma}_{\textbf{Impurity}} + \underbrace{\sum_\alpha \gamma_\alpha (b^\dagger_{\alpha\sigma} c_\sigma + c^\dagger_\sigma b_{\alpha\sigma})}_{\textbf{Hybridization}}$$

bs are the bath states, ϵ_α and γ_α, and even α's themselves are unknows as of now!

- **This type of a problem is called a "Quantum Impurity Problem", the specific one above is called the "Anderson Impurity Problem"**
- **Key point to note is that only "interacting piece" in the above Hamiltonian occurs only on the impurity**
- **Lots of unknowns at this point...ϵ_α, γ_α!**

DMFT - Key Ideas

- **Assume that we somehow know ϵ_α and γ_α**
- **Suppose U were zero, then we can solve the problem exactly (quadratic Hamiltonian!), and obtain the Green's function of the impurity $\mathcal{G}_\sigma(i\omega_n)$**
- **Note that $\mathcal{G}_\sigma(i\omega_n)$ has *all* the *required* information regarding ϵ_α and γ_α...i. e., this is what we take that we *know***
- **Key question: Suppose $\mathcal{G}_\sigma(i\omega_n)$ is given, what is the Green's function with $U \neq 0$? The "thing" that gives us the answer to this question is the "impurity solver"!**
- **Upshot: We specify the bath by $\mathcal{G}_\sigma(i\omega_n)$, for a given U, the impurity solver will give us the Green's function $G_\sigma(i\omega_n)$ (and of course $\Sigma_\sigma(i\omega_n)$)**

DMFT - Key Ideas

- **We now take the next step...**
- **The** *DMFT Ansatz* **: Assert that** $\Sigma(\boldsymbol{k}\sigma, i\omega_n) = \Sigma_\sigma(i\omega_n)$**! This is a statement that is rigrously true in** *infinite* **dimensions or on a lattice with** *infinite* **coordination...**
- **Recall what our elders told us...be happy with what you have...for us** $d = 2, 3$**, and we take it to be infinity!**
- **This now allows us to calculate the** *Lattice* **Green's function of the site** i **as**

$$G_{i\sigma}(i\omega_n) = \frac{1}{N}\sum_{\boldsymbol{k}} \frac{1}{i\omega_n - \varepsilon(\boldsymbol{k}) + \mu - \Sigma_\sigma(i\omega_n)}$$

This is where all the information about the lattice etc. goes...

DMFT - Key Ideas

- **We now take the final step!**
- **We now know $G_{i\sigma}(i\omega_n)$ and $\Sigma_\sigma(i\omega_n)$...what happens if we "remove the self energy effects due to interactons" from $G_{i\sigma}(i\omega_n)$, i. e., what is**

$$G^{-1}_{i\sigma}(i\omega_n) + \Sigma_\sigma(i\omega_n)?$$

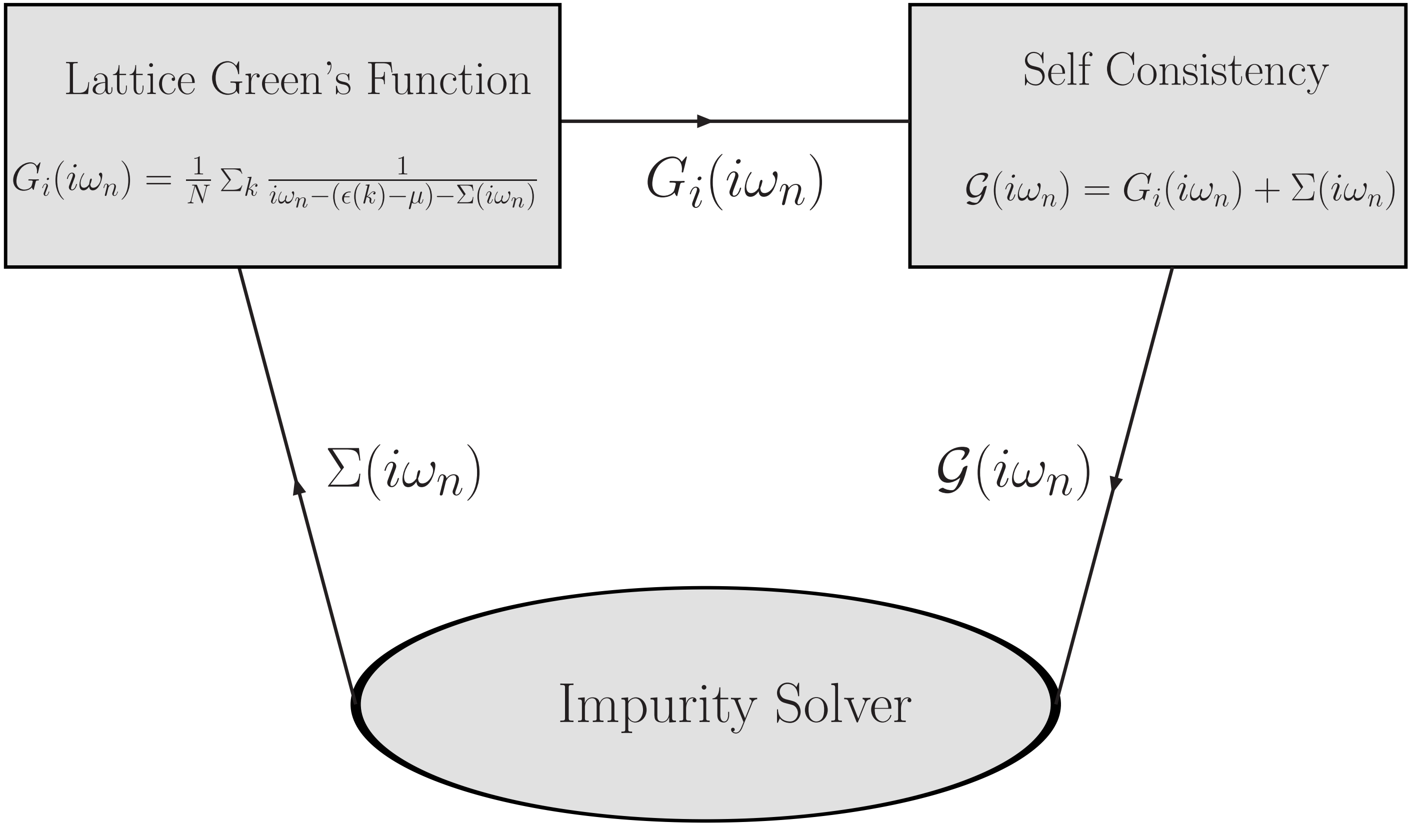
- **This** *must* **be "mixing" with the rest of the lattice, i. e.,**

$$G^{-1}_{i\sigma}(i\omega_n) + \Sigma_\sigma(i\omega_n) = \mathcal{G}_\sigma(i\omega_n)$$

- **Thus we get information about the bath! Note that everything on the LHS is determined by the bath which is specified by $\mathcal{G}_\sigma$, and therefore the above equation is the** *self consistency* **equation!**

DMFT - Summary

- **We can now develop an iterative scheme to solve the self consistency equation...**



Lattice Green's Function

$$G_i(i\omega_n) = \frac{1}{N}\sum_k \frac{1}{i\omega_n - (\epsilon(k) - \mu) - \Sigma(i\omega_n)}$$

$G_i(i\omega_n)$

Self Consistency

$$\mathcal{G}(i\omega_n) = G_i(i\omega_n) + \Sigma(i\omega_n)$$

$\mathcal{G}(i\omega_n)$

Impurity Solver

$\Sigma(i\omega_n)$

- **The most difficult step is the impurity solution...**

Quantum Impurity Solvers

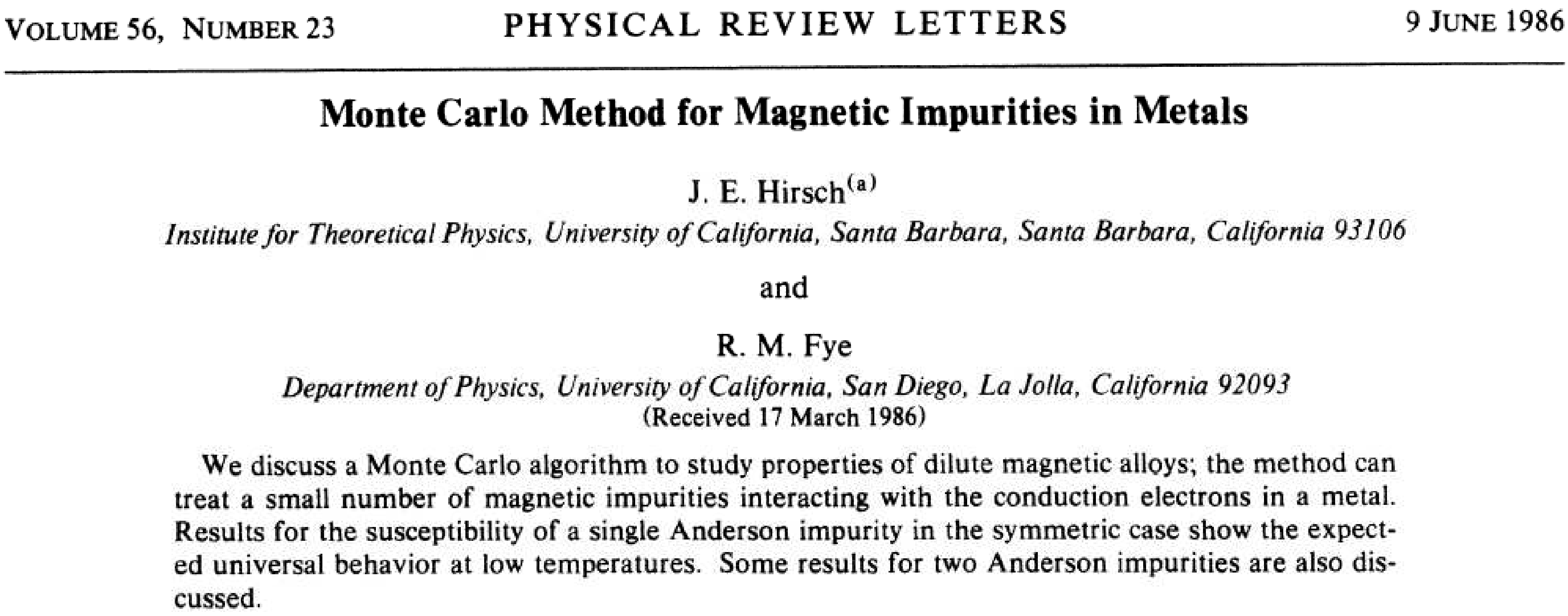
- Analytical/Semi-analytical
  - Iterated Perturbation Theory
  - Non-crossing approximation
  - Local-moment approach
  - etc.
- Numerical approaches
  - Exact diagonalization
  - Quantum Monte Carlo (QMC)
  - Numerical renormalization group (NRG)
  - Density-matrix renormalization group (DMRG)
- Our focus QMC, and ideas of NRG if time permits...

What is the difficulty?

- The physics we are interested in happens at very small energy scales
- But the physics at small energy scales is strongly affected by the larger scales!
- How to handle all the scales involved?

Hirsch-Fye Quantum Monte Carlo

- **Based on ideas of Blackenbecler, Scalapinio and Sugar (1981)**



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Monte Carlo Method for Magnetic Impurities in Metals

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We discuss a Monte Carlo algorithm to study properties of dilute magnetic alloys; the method can treat a small number of magnetic impurities interacting with the conduction electrons in a metal. Results for the susceptibility of a single Anderson impurity in the symmetric case show the expected universal behavior at low temperatures. Some results for two Anderson impurities are also discussed.

- **We will now keep DMFT aside, and learn how to solve the Anderson impurity problem with HF-QMC**

Hirsch-Fye Quantum Monte Carlo

- **Input:** $\mathcal{G}_\sigma(\tau)$, **Output :** $G_\sigma(\tau)$
- **Key steps**
  - **Perform Trotter decomposition of the partition function – L times slices**
  - **Introduce** *discrete* **Ising spin like Hubbard-Stratanovic fields at every time slice for the interaction at the impurity**
  - **The problem now has the quadratic electronic degrees of freedom and the Ising spins at the impurity site for every time slice**
  - **Integrate out the electrons to obtain the partition function in terms of the Ising spins**
  - **Perform Monte Carlo moves involving flips of Ising spins to calculate observables**

HF-QMC: Preliminaries

- We now change notation a bit...
- Imagine that the impurity and bath together contain a total of M sites, the first one is the impurity, and the others are bath sites

$$\begin{aligned}\mathcal{H} &= \underbrace{(\frac{U}{2}-\mu)(n_\uparrow+n_\downarrow)+\sum_{j=2}^{M}\varepsilon_j c^\dagger_{j\sigma}c_{j\sigma}+\sum_{j=2}^{M}\gamma_j\left(c^\dagger_{j\sigma}c_\sigma+c^\dagger_\sigma c_{j\sigma}\right)}_{\mathcal{H}_0-\textbf{Noninteracting part}}\\ &\quad \underbrace{+U\left(n_\uparrow n_\downarrow-\frac{1}{2}(n_\uparrow+n_\downarrow)\right)}_{\mathcal{U}-\textbf{Interacting part}}\end{aligned}$$

- We have dropped A subscript on the Hamiltonian, c_σ with out a j stands for the impurity i.e., $j=1$ etc.
- Notation for quadratic operators, we write $\mathcal{A}=\sum_{ij}\mathbb{A}_{ij}c^\dagger_{i\sigma}c_{j\sigma}$ where $\mathbb{A}$ is a matrix

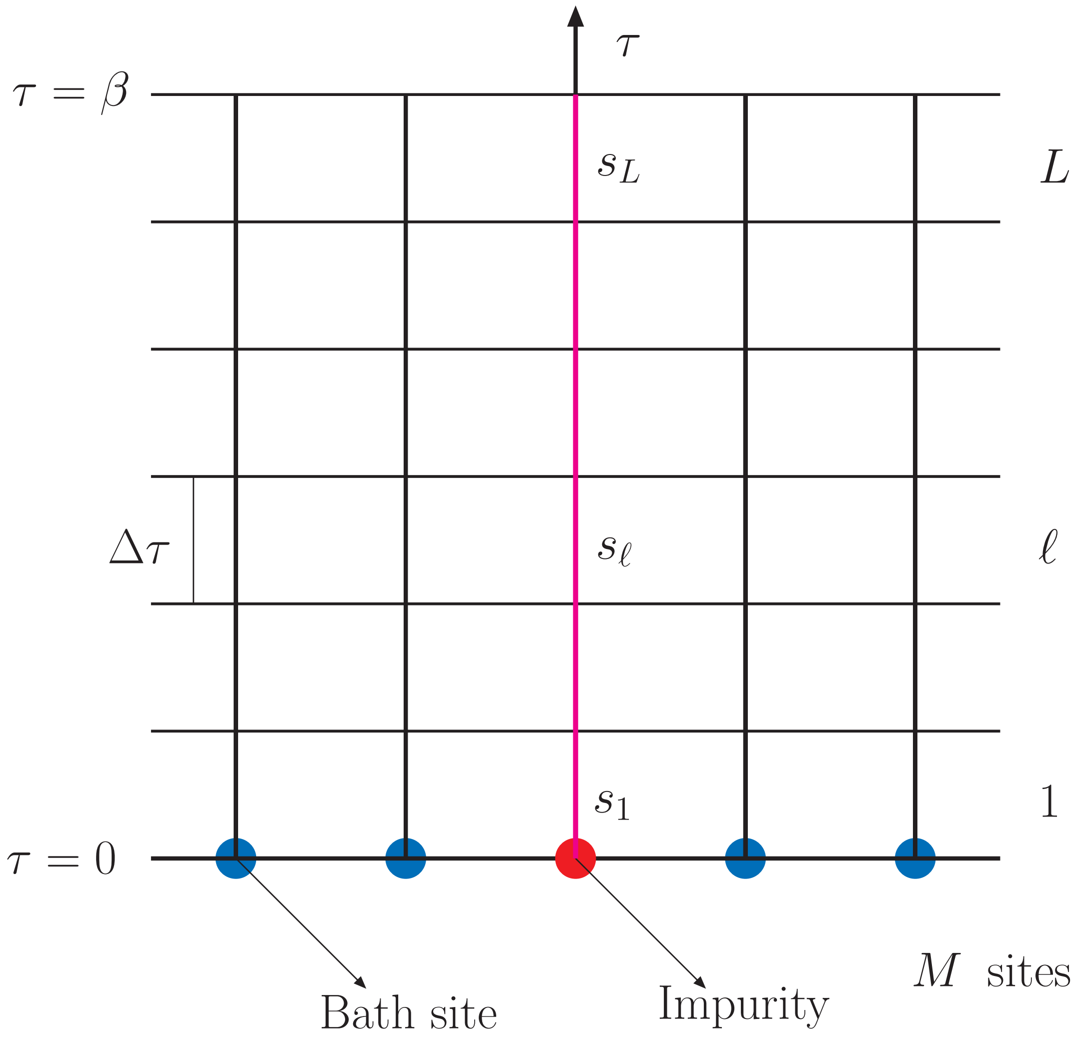
HF-QMC: Times Slices

- **Aim is to calculate the partition function** $Z = \mathrm{Tr} e^{-\beta \mathcal{H}}$
- **We introduce** L **slices on the imaginary time axis each of width** $\Delta\tau = \frac{\beta}{L}$
- **The partition function is then written as**

$$Z = \mathrm{Tr} \left(\prod_{\ell=1}^{L} e^{-\Delta\tau \mathcal{H}} \right)$$

- **So far there is no approximation of any kind!**

HF-QMC: Times Slices



HF-QMC: Trotter-Suzuki Approximation

- Consider $e^{-\Delta\tau\mathcal{H}} = e^{-\Delta\tau(\mathcal{H}_0+\mathcal{U})}$
- Note that $\mathcal{U}$ does not commute with $\mathcal{H}_0$
- We can approximate

$$e^{-\Delta\tau(\mathcal{H}_0+\mathcal{U})} = e^{-\Delta\tau\mathcal{H}_0} e^{-\Delta\tau\mathcal{U}} + O(\Delta\tau^2)$$

This does introduce a systematic error, which can be taken to zero by making $\Delta\tau \longrightarrow 0$...this is the only source of systematic error in this method

- With this approximation

$$Z = \mathrm{Tr}\left(\prod_{\ell=1}^{L} e^{-\Delta\tau\mathcal{H}_0} e^{-\Delta\tau\mathcal{U}}\right)$$

QMC: Hirsch-Hubbard-Stratanovic Transformat

- We now use the identity

$$e^{-\Delta\tau\mathcal{U}} = \frac{1}{2}\sum_{s=\pm 1} e^{\lambda s(n_\uparrow - n_\downarrow)}$$

if λ is chosen such that

$$e^{\Delta\tau\frac{U}{2}} = \cosh(\lambda)$$

- Idea of the proof: the Hilbert space of the impurity is spanned by states $|00\rangle, |\uparrow 0\rangle, |0\downarrow\rangle, |\uparrow\downarrow\rangle$, these states are eigenstates of both LHS and RHS operators, if λ is chosen appropriately

QMC: Hirsch-Hubbard-Stratanovic Transformat

- **Now take the term $e^{-\Delta\tau\mathcal{U}}$ in the ℓ-th time slice and use the HHS identity to get**

$$e^{-\Delta\tau\mathcal{U}}\Big|_{\ell} = \frac{1}{2}\sum_{s_\ell} e^{\lambda s_\ell (n_\uparrow - n_\downarrow)}$$

- **Note that exponential in the right hand side is a** *quadratic* **operator...thus it is "as if" the impurity is experiencing a** *one body* **potential from the auxillary ising spin field...**

QMC: Hirsch-Hubbard-Stratanovic Transformat

- **We can therefore define a quadratic operator $\mathcal{V}_\sigma(\ell)$ which depends on the Ising spin configuration at the slice ℓ**

$$\mathcal{V}_\sigma(\ell) = \sum_{i,j} (\mathbb{V}_\sigma(\ell))_{ij} c^\dagger_{i\sigma} c_{j\sigma}; \;\; \mathbb{V}_\sigma = \begin{pmatrix} \sigma\lambda s_\ell & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix}_{M \times M}$$

- **Thus the stuff at the ℓ-th time slice in the partition function can now be written as** **Question: Why?**

$$e^{-\Delta\tau\mathcal{H}_0} e^{-\Delta\tau\mathcal{U}}\Big|_\ell = \frac{1}{2}\sum_{s_\ell} e^{-\Delta\tau\mathcal{H}_{0\uparrow}} e^{\mathcal{V}_\uparrow(\ell)} e^{-\Delta\tau\mathcal{H}_{0\downarrow}} e^{\mathcal{V}_\downarrow(\ell)}$$

-QMC: Partition Function in Terms of Ising spi

- **Now the partition function can be written as**

$$Z = \left(\frac{1}{2}\right)^L \sum_{\{s_1,\ldots,s_L\}} \mathrm{Tr}\left(\prod_{\ell=1}^{L} e^{-\Delta\tau\mathcal{H}_{0\uparrow}} e^{\mathcal{V}_\uparrow(\ell)} e^{-\Delta\tau\mathcal{H}_{0\downarrow}} e^{\mathcal{V}_\downarrow(\ell)}\right)$$

- **This can be recast as** **Question: Why?**

$$Z = \left(\frac{1}{2}\right)^L \sum_{\{s_1,\ldots,s_L\}} \mathrm{Tr}\left(\prod_{\ell=1}^{L} e^{-\Delta\tau\mathcal{H}_{0\uparrow}} e^{\mathcal{V}_\uparrow(\ell)}\right) \mathrm{Tr}\left(\prod_{\ell=1}^{L} e^{-\Delta\tau\mathcal{H}_{0\downarrow}} e^{\mathcal{V}_\downarrow(\ell)}\right)$$

- **If we can perform the traces, we see that the partition function can be written as**

$$Z = \sum_{\{s_1,\ldots,s_L\}} \textbf{some function of} \{s_1,\ldots,s_L\}$$

We have achieved our goal *in principle*; **we now evaluate the "some function"**

HF-QMC: Two Lemmas

- **Lemma I: Let $\mathcal{A} = \sum_{ij} \mathbb{A}_{ij} c_i^\dagger c_j$ Question: Why are there no spin indices?, then**

$$\mathrm{Tr} e^{-\mathcal{A}} = \det\left(\mathbf{1} + e^{-\mathbb{A}}\right)$$

Proof is quite easy...

- **Lemma II: Consider quadratic operators $\mathcal{A}, \mathcal{B}, \mathcal{C} \ldots$, then**

$$\mathrm{Tr}(e^{-\mathcal{A}} e^{-\mathcal{B}} e^{-\mathcal{C}} \ldots) = \det\left(\mathbf{1} + e^{-\mathbb{A}} e^{-\mathbb{B}} e^{-\mathbb{C}} \ldots\right)$$

HF-QMC: The Partition Function

- **With these lemmas, we can write**

$$\begin{aligned} Z &= \sum_{\{s_1,\ldots,s_L\}} \det\left(\mathbf{1} + e^{-\Delta\tau\mathbb{H}_0} e^{\mathbb{V}_\uparrow(1)} \ldots e^{-\Delta\tau\mathbb{H}_0} e^{\mathbb{V}_\uparrow(\ell)} \ldots e^{-\Delta\tau\mathbb{H}_0} e^{\mathbb{V}_\uparrow(L)}\right) \times \\ & \det\left(\mathbf{1} + e^{-\Delta\tau\mathbb{H}_0} e^{\mathbb{V}_\uparrow(1)} \ldots e^{-\Delta\tau\mathbb{H}_0} e^{\mathbb{V}_\uparrow(\ell)} \ldots e^{-\Delta\tau\mathbb{H}_0} e^{\mathbb{V}_\uparrow(L)}\right) \end{aligned}$$

Question: What has been dropped? Is it okay?

- **Now following the standard route, we define matrices**

$$\mathbb{B}_\sigma(\ell) = e^{-\Delta\tau\mathbb{H}_{0\sigma}} e^{\mathbb{V}_\sigma(\ell)}$$

to get

$$Z = \sum_{\{s_1,\ldots,s_L\}} \det\left(\mathbf{1} + \mathbb{B}_\uparrow(L)\ldots\mathbb{B}_\uparrow(\ell)\ldots\mathbb{B}_\uparrow(1)\right) \det\left(\mathbf{1} + \mathbb{B}_\downarrow(L)\ldots\mathbb{B}_\downarrow(\ell)\ldots\mathbb{B}_\downarrow(1)\right)$$

HF-QMC: The Partition Function

- **Now with a little bit of matrix algebra one can show that**

$$\det\left(\mathbf{1} + \mathbb{B}_\sigma(L)\ldots\mathbb{B}_\sigma(\ell)\ldots\mathbb{B}_\sigma(1)\right) = \det \mathscr{O}_\sigma(\{s_\ell\})$$

where

$$\mathscr{O}_\sigma(\{s_\ell\}) = \begin{pmatrix} \mathbf{1} & \mathbf{0} & \mathbf{0} & \ldots & \mathbf{0} & \mathbb{B}_\sigma(L) \\ -\mathbb{B}_\sigma(1) & \mathbf{1} & \mathbf{0} & \ldots & \ldots & \mathbf{0} \\ \mathbf{0} & -\mathbb{B}_\sigma(2) & \mathbf{1} & \mathbf{0} & \ldots & \mathbf{0} \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & -\mathbb{B}_\sigma(L-2) & \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \ldots & \ldots & \ldots & -\mathbb{B}_\sigma(L-1) & \mathbf{1} \end{pmatrix}_{ML\times ML}$$

which is an $L \times L$ matrix of $M \times M$ matrices

HF-QMC: The Partition Function

- **The partition function is now**

$$Z = \sum_{\{s_1,\ldots,s_L\}} \det \mathscr{O}_\uparrow(\{s_\ell\}) \det \mathscr{O}_\downarrow(\{s_\ell\})$$

- **In particular** *any Fermionic observable* A **can be calculated** *for a given Ising spin* **configuration as** $A(\{s_\ell\})$ **by Wick's theorem**

$$\langle A \rangle = \sum_{\{s_1,\ldots,s_L\}} A(\{s_\ell\}) \frac{\det \mathscr{O}_\uparrow(\{s_\ell\}) \det \mathscr{O}_\downarrow(\{s_\ell\})}{Z}$$

- **We can now interpret** $\det \mathscr{O}_\uparrow(\{s_\ell\}) \det \mathscr{O}_\downarrow(\{s_\ell\})/Z$ **as the** *statistical weight* **of the Ising spin configuration!**

HF-QMC: The Algorithm

- **This will be perfectly fine if** $\det \mathscr{O}_\uparrow(\{s_\ell\}) \det \mathscr{O}_\downarrow(\{s_\ell\})$ **is of the same sign for all Ising spin configurations! It is empirically known (and recently proved) that there is** *no sign problem* **(unless you ask for the unreasonable)**
- **Note that we have mapped a quantum impurity problem to one of an chain of Ising spins of length** L**!** d**-Quantum** $= d+1$**-Classical!**
- **The QMC Algo**
  - **Start with a random Ising spin configuration** $\{s_\ell\}$
  - **Visit each Ising spin and attempt to flip it by calculating the ratio of the weights of the configuration, i. e., if you attempt to do** $\{s_\ell\} \longrightarrow \{s'_\ell\}$**, you have to calculate**

$$r = \frac{\det \mathscr{O}_\uparrow(\{s'_\ell\}) \det \mathscr{O}_\downarrow(\{s'_\ell\})}{\det \mathscr{O}_\uparrow(\{s_\ell\}) \det \mathscr{O}_\downarrow(\{s_\ell\})}$$

  - **Accept or reject** $\{s'_\ell\}$ **based on** r

HF-QMC: Some Questions

- **At this stage it appears that one has to calculate determinants of an $ML \times ML$ matrices to perform the Ising spin update!**
- **There are further problems...Actually, we** *do not know* **all the details of the bath!, we know only the Green's function $\mathcal{G}$**
- **....**
- **How do we proceed?**
- **In fact, whatever we have discussed so far was developed by Blackenbecler, Scalapino and Sugar...Hirsch and Fye made some key observations which make this possible...**

HF-QMC: Key Obsevations

- **What is the "meaning" of the matrix $\mathscr{O}_\sigma(\{s_\ell\})$?**
- **A little thought will tell you that $\mathscr{G}_\sigma(\{s_\ell\}) = \mathscr{O}_\sigma^{-1}(\{s_\ell\})$, the Green's function of** *impurity + bath* **for** *a given realization of the Ising spin configuration!*
- **In particular, if i and j are any two sites in the system,**

$$(\mathscr{G}_\sigma(\{s_\ell\}))_{(\ell_1,i);(\ell_2,j)} = \langle c_{i\sigma}(\ell_1) c^\dagger_{j\sigma}(\ell_2)\rangle_{\{s_\ell\}}, \quad \ell_1 > \ell_2$$

- **Specifically,**

$$(G_\sigma(\{s_\ell\}))_{\ell_1,\ell_2} = (\mathscr{G}_\sigma(\{s_\ell\}))_{(\ell_1,1);(\ell_2,1)} = \langle c_\sigma(\ell_1) c^\dagger_\sigma(\ell_2)\rangle_{\{s_\ell\}}, \quad \ell_1 > \ell_2$$

is the *impurity Green's function* **for a given realization of the Ising spin configuration! $G_\sigma(\{s_\ell\})$ is an $L \times L$ sub-matrix of $\mathscr{G}_\sigma(\{s_\ell\})$**

HF-QMC: Key Obsevations

- $\mathscr{G}_\sigma(\{s_\ell\})$ **depends on the Ising spin configuration $\{s_\ell\}$...Hirsch and Fye made the key observation that if the spin configuration is changed to $\{s'_\ell\}$, then the new $\mathscr{G}_\sigma(\{s'_\ell\}) = \mathscr{G}'_\sigma$ satisfies a Dyson like equation**

  $$\mathscr{G}'_\sigma = \mathscr{G}_\sigma + (\mathscr{G}_\sigma - 1)e^{\mathscr{V}_\sigma - \mathscr{V}'_\sigma}\mathscr{G}'_\sigma$$

  where 1 is a $ML \times ML$ identity, and $\mathscr{V}$ is an $ML \times ML$ diagonal matrix

  $$(\mathscr{V}_\sigma)_{(\ell_1,i);(\ell_2,j)} = \delta_{i,1}\delta_{j,1}\delta_{\ell_1,\ell_2}\,\sigma\lambda s_{\ell_1}$$

- **There is more...**

HF-QMC: Key Obsevations

- **Here is the** *punch line* **observation of Hirsch-Fye...**
- **The new** *impurity* **Green's function matrix** G'_σ *also* **satisfies a Dyson equation of the form**

$$G'_\sigma = G_\sigma + (G_\sigma - \mathbf{1})e^{V - V'} G'_\sigma$$

where $\mathbf{1}$ **is a** $L \times L$ **identity, and** $\mathscr{V}$ **is an** $L \times L$ **diagonal matrix**

$$(V_\sigma)_{\ell_1 \ell_2} = \delta_{\ell_1, \ell_2} \sigma \lambda s_{\ell_1}$$

- **Suddenly, we realize** **Question: How?**

$$G_\sigma = \mathcal{G}_\sigma + (\mathcal{G}_\sigma - \mathbf{1})e^{-V} G_\sigma$$

HF-QMC: Key Obsevations

- **Thus if we know $\mathcal{G}$ (which we do!), we can calculate G_σ which depends on the Ising spin configuration!**
- **And, here is the final observation**

$$\frac{\det \mathscr{O}'_\sigma}{\det \mathscr{O}_\sigma} = \frac{\det G_\sigma}{\det G'_\sigma}$$

- **Happily, now**
  - **We need to worry only about $L \times L$ determinants!**
  - **We need only $\mathcal{G}$!**
- **A couple of more technical things...**

HF-QMC: Key Obsevations

- **Note when we go from spin configuration s to s' we flip the spin *only* at one τ-site, say ℓ...**
- **It turns out that we can *explicitly* calculate the ratio of the determinants**

$$\frac{\det G_\sigma}{\det G'_\sigma} = 1 + (1 - (G_\sigma)_{\ell\ell})(e^{-2\lambda\sigma s_\ell} - 1)$$

...as simple as that! Just one floating multiplication!!

- **If the new configuration is accepted, then we have to update G_σ...there is an $L \times L$ efficient formula**

$$(G'_\sigma)_{\ell_1\ell_2} = (G_\sigma)_{\ell_1\ell_2} + \frac{(G_\sigma)_{\ell_1\ell}(e^{-2\lambda\sigma s_\ell} - 1)(G_\sigma)_{\ell\ell_2}}{1 + (1 - (G_\sigma)_{\ell\ell})(e^{-2\lambda\sigma s_\ell} - 1)}$$

HF-QMC: The Complete Algorithm

- **Input, the matrix $\mathcal{G}$, choose L**
- **Generate a random string of Ising spins $\{s_\ell\}$; set up G using $G_\sigma = \mathcal{G}_\sigma + (\mathcal{G}_\sigma - 1)e^{-V}G_\sigma$**
- **Visit each Ising spin, calculate r**
- **If the new configuration is accepted, update the Green's function using the L^2 update**
- **Keep track of observables**
- **...**
- **The only point to be noted is that we need to make sure that the precision is maintained, so every so often, we use the L^3 formula to generate the Green's function**

F-QMC Example : Anderson Impurity Problem

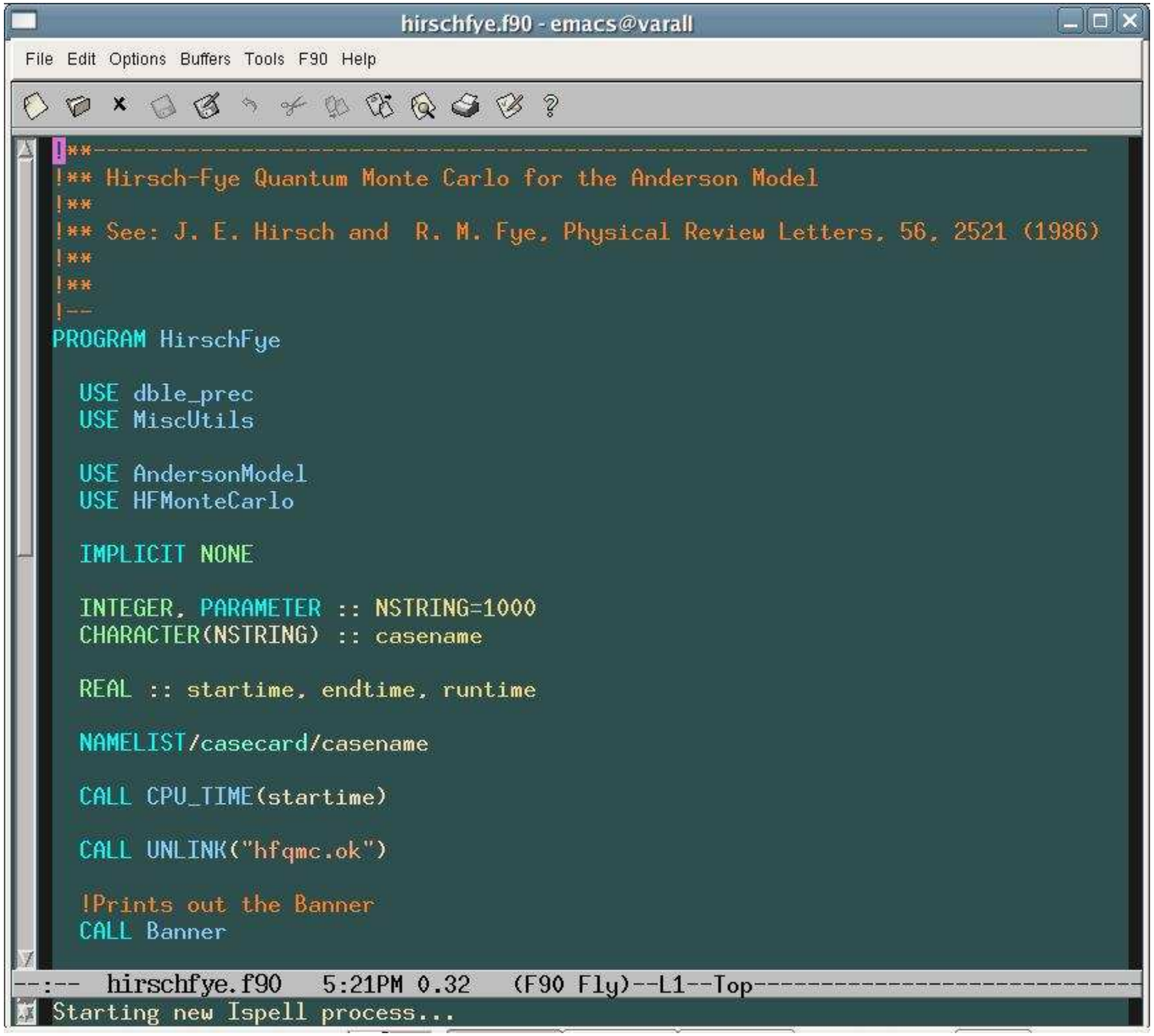
- **The Anderson impurity problem is specified by three parameters**
  1. ε_d – d-**orbital (imipurity) energy level**
  2. Δ – **effective hybridization parameter**
  3. U – **Coulomb repulsion**
- **The bare Greens function** $\mathcal{G}$ **can be explicitly calculated as**

$$\mathcal{G}_\sigma(\tau) = \int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{e^{-\omega\tau}}{e^{-\beta\omega}+1} \, \frac{1}{\pi} \frac{\Delta}{(\omega - \varepsilon_d - U/2)^2 + \Delta^2}$$

- **For the symmetric model** $\varepsilon_d = -U/2$, **the Kondo temperature is** $T_K \sim \sqrt{\frac{\Delta}{U}} e^{-\frac{\pi U}{8\Delta}}$

F-QMC Example : Anderson Impurity Problem

- **HFQMC code – freely available with this lectures**

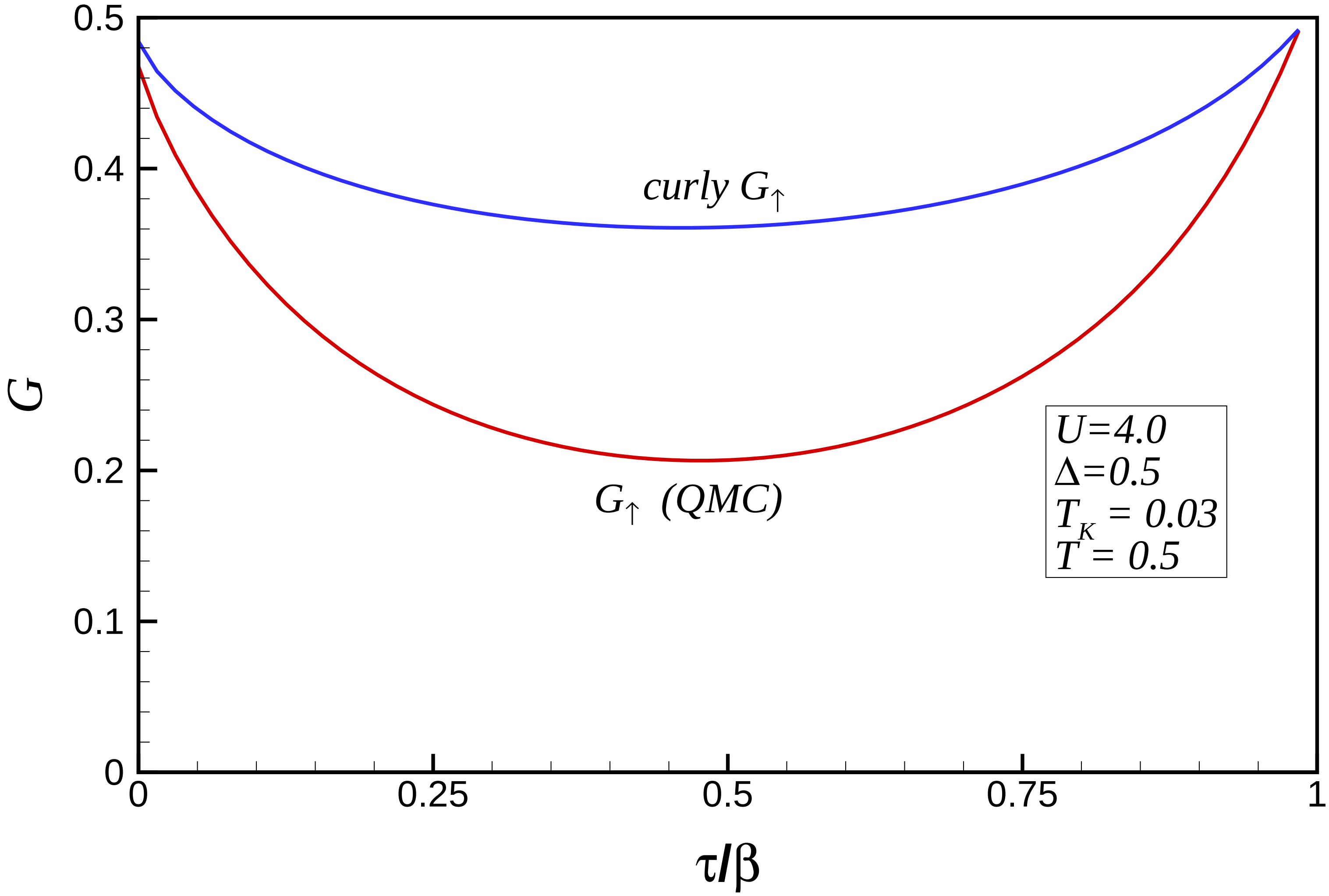


```
!**-----------------------------------------------------------------------
!** Hirsch-Fye Quantum Monte Carlo for the Anderson Model
!**
!** See: J. E. Hirsch and  R. M. Fye, Physical Review Letters, 56, 2521 (1986)
!**
!**
!--
PROGRAM HirschFye

  USE dble_prec
  USE MiscUtils

  USE AndersonModel
  USE HFMonteCarlo

  IMPLICIT NONE

  INTEGER, PARAMETER :: NSTRING=1000
  CHARACTER(NSTRING) :: casename

  REAL :: startime, endtime, runtime

  NAMELIST/casecard/casename

  CALL CPU_TIME(startime)

  CALL UNLINK("hfqmc.ok")

  !Prints out the Banner
  CALL Banner
```

```
--:--  hirschfye.f90    5:21PM 0.32    (F90 Fly)--L1--Top-------------------------
Starting new Ispell process...
```

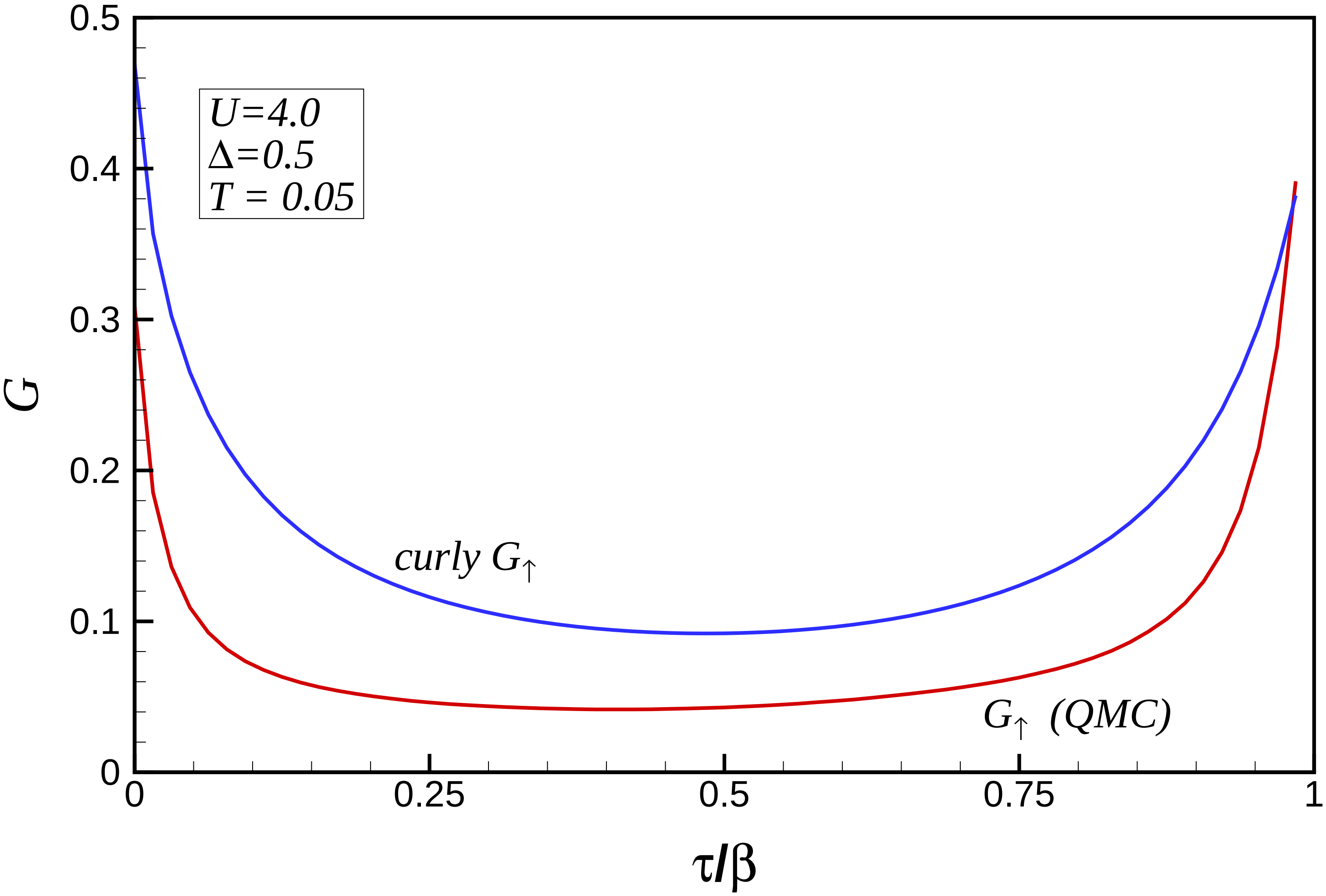
F-QMC Example : Anderson Impurity Problem

- **System with** $T_K = 0.03$



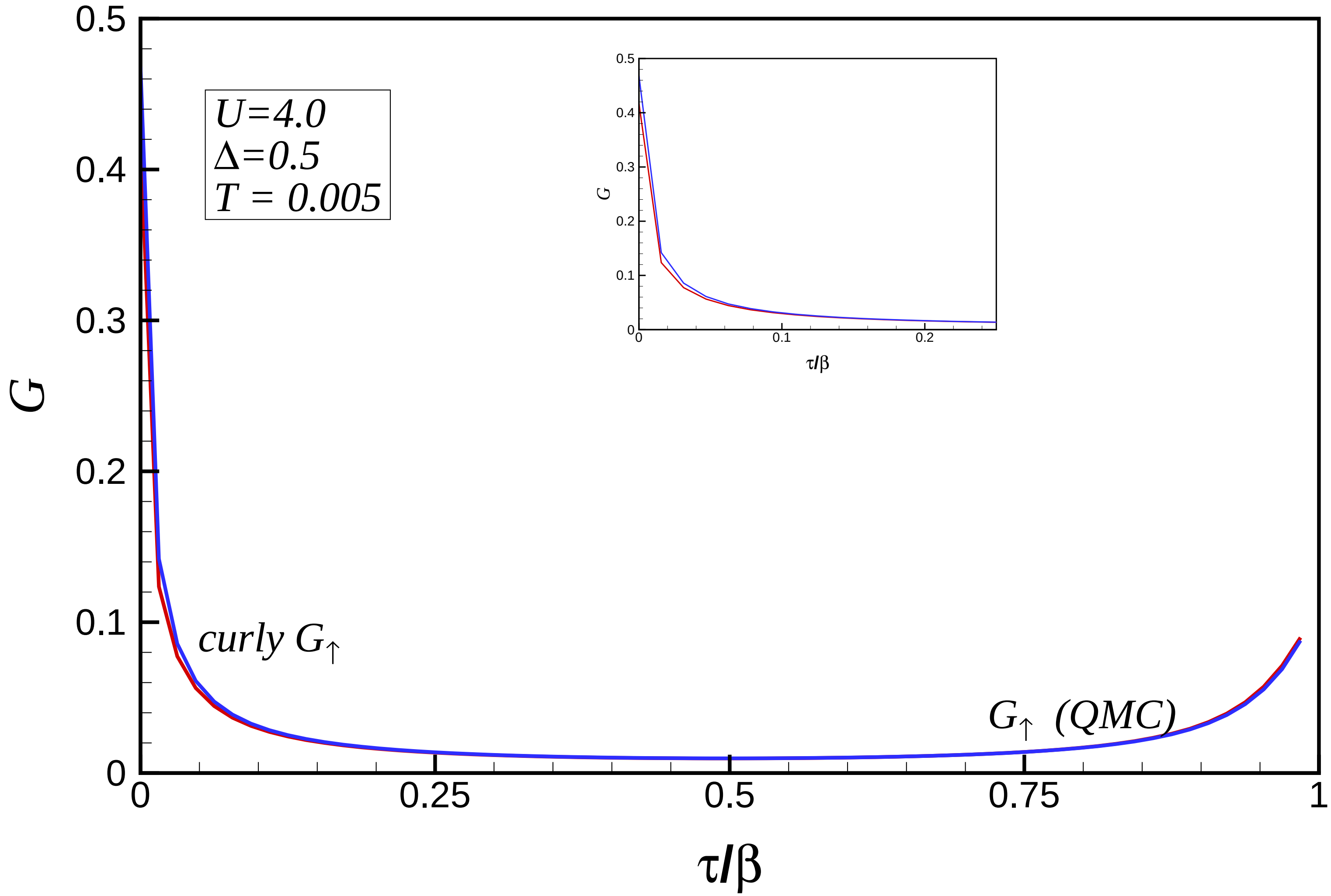
F-QMC Example : Anderson Impurity Problem

- **System with** $T_K = 0.03$



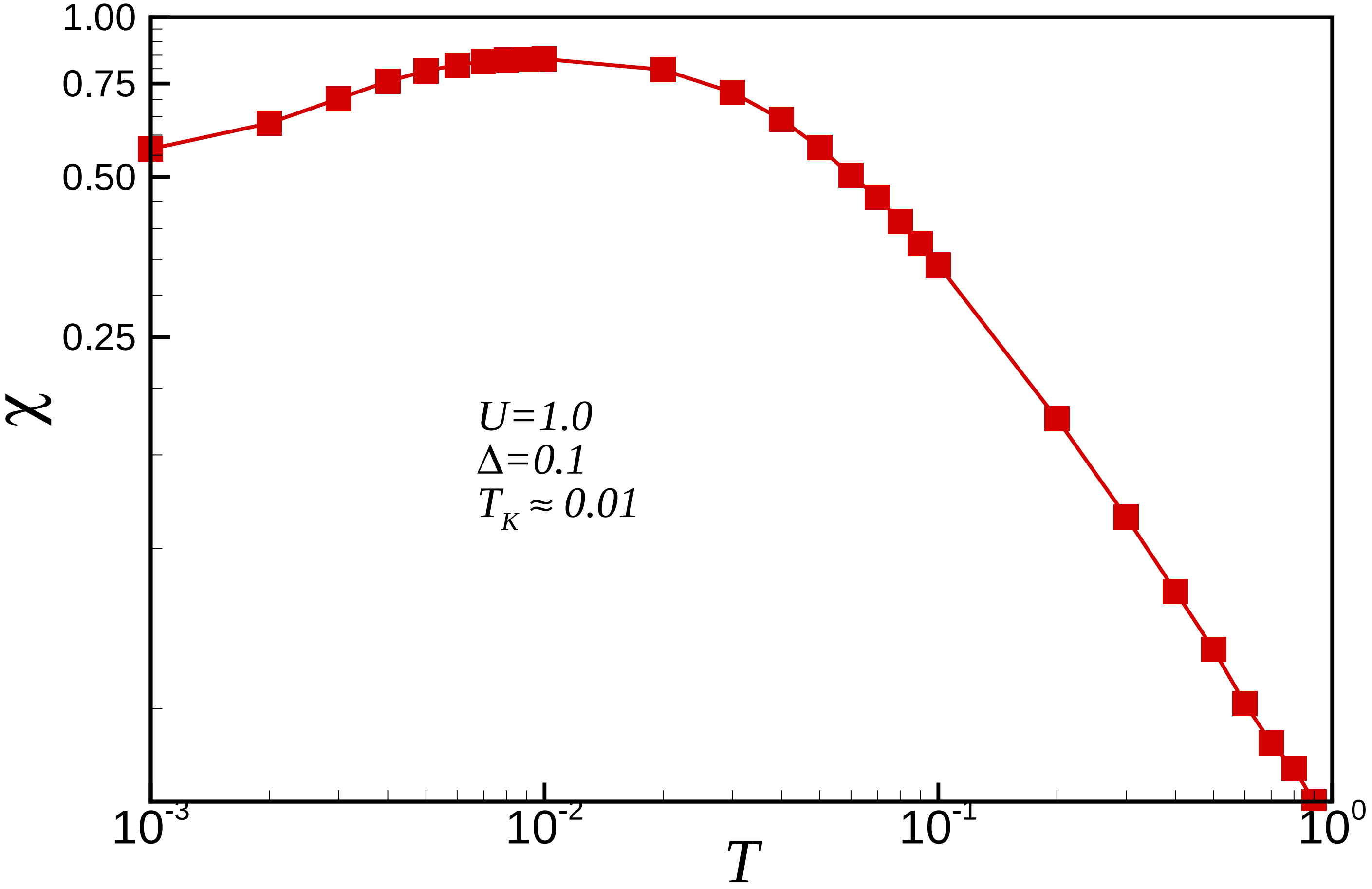
F-QMC Example : Anderson Impurity Problem

- **System with** $T_K = 0.03$



F-QMC Example : Anderson Impurity Problem

- **Susceptibility**



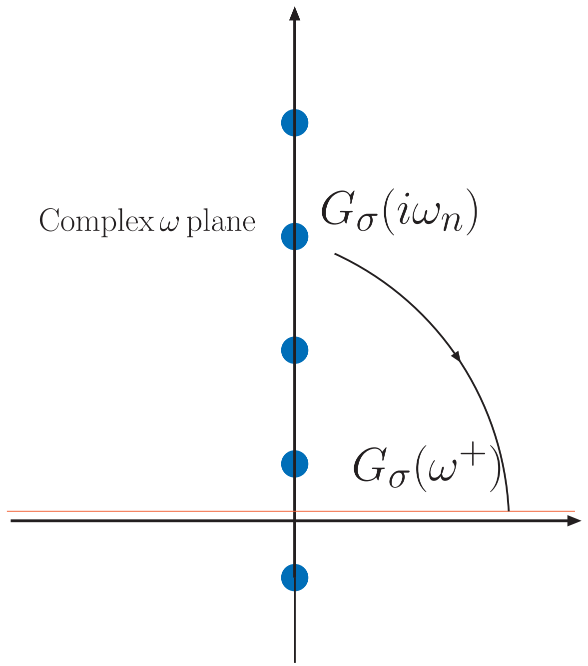
- **What is the physics?**

HF-QMC and DMFT

- **Once we obtain $G_\sigma(\tau)$ we can calculate $G_\sigma(i\omega_n)$**
- **Calculate $\Sigma_\sigma(i\omega_n)$ using Dyson equation**
- **Feed $\Sigma_\sigma(i\omega_n)$ to the lattice etc...**
- **...**
- **Iterate to convergence**
- **...**
- **We need physical quantities such as $A_\sigma(\omega)$...what we have is $G_\sigma(\tau)$ or equivalently $G_\sigma(i\omega_n)$**

Analytical Continuation

- **We have information along the discrete Matsubara frequencies in $G_\sigma(i\omega_n)$ (or equivalently $G_\sigma(\tau)$)**



- **Several ideas around**
  - **Padé approximation**
  - **Maximum entropy method**

Padé Approximation

- **Pre-DMFT, used in strong coupling superconductivity (Vidberg and Serene 1977)**
- **The idea is simple: "Fit a rational function to data", i. e.,**

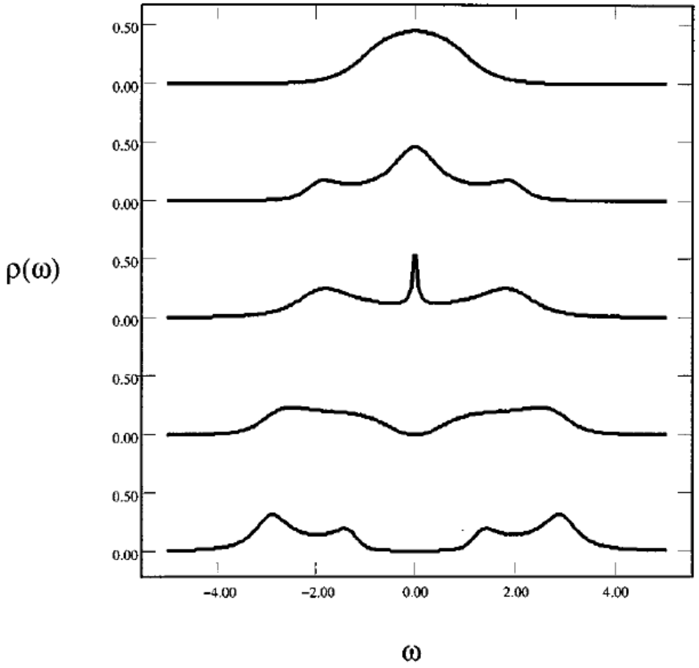
$$G_\sigma(\omega) = \frac{P_n(\omega)}{R_m(\omega)}$$

where P_n, R_m are polynomials of degrees n and m

- **We now determine the polynomials from the known $G_\sigma(i\omega_n)$... The nice thing is that this allows for $poles$ which have physical significance**

Padé Approximation

- $G_\sigma(\tau)$ **obtained by** *exactly summing* **the partition function**



Georges et al. RMP, 1996, Note how a Mott insulator emerges with increasing U

- **Problem: Small errors (such as statistical errors) in G_σ can give very wild answers! Ill-posed!**

Maximum Entropy

- **Digression: We have a dice on which we do an experiment, and find that the mean is 4... we ask what is the probability p_i of getting face i**
- **We know $\sum_i x_i p_i = \bar{x} = 4$**
- **We also know $\sum_i p_i = 1$**
- **How can we find p_i? Shanonn's solution: Maximize the** *information entropy* $S[p] = -\sum_i p_i \ln p_i$
- **We maximize $S[p]$ subject to the known conditions**

Maximum Entropy

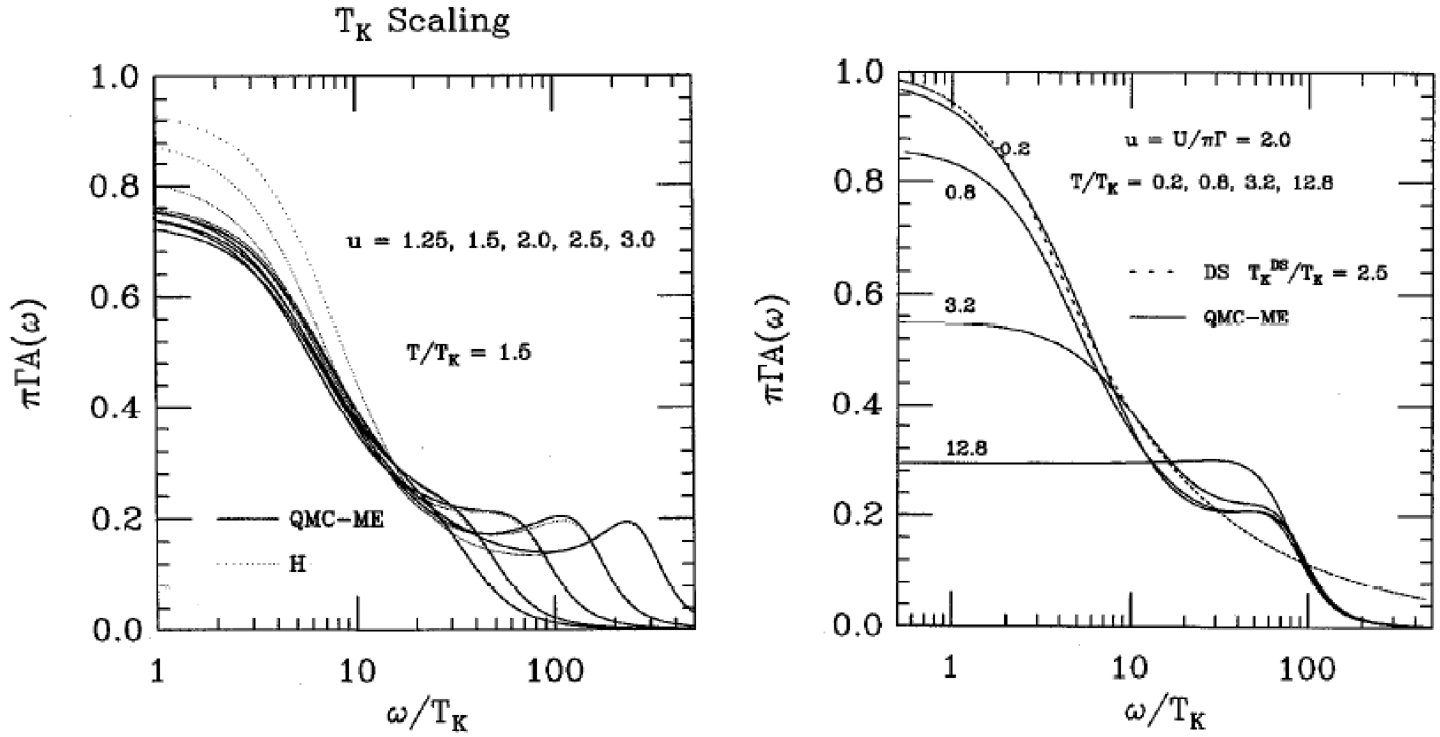
- **Back to our problem, we know $G_\sigma(\tau)$ for a discrete set of values**
- **This is related to $A_\sigma(\omega)$ by**

$$G_\sigma(\tau) = \int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{e^{-\omega\tau}}{e^{-\beta\omega} + 1} \, A_\sigma(\omega)$$

- **Also we know that $\int_{-\infty}^{\infty} \mathrm{d}\omega A(\omega) = 1$**
- **Information entropy $S[A] = -\int_{-\infty}^{\infty} \mathrm{d}\omega A(\omega) \ln A(\omega)$**
- **Maximize $S[A]$, with knowledge of the errors in the QMC (Gubernatis et al. 1991)**

Maximum Entropy

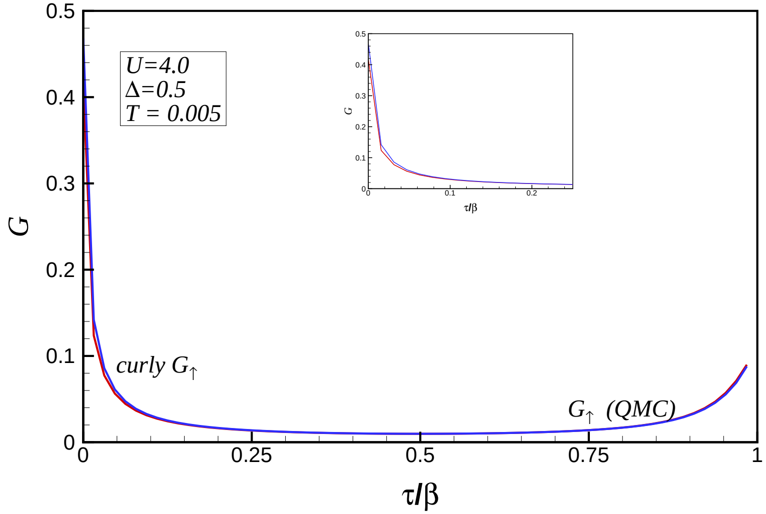
- **Solution of the Anderson impurity problem**



Jarrell and Gubernatis, Phys. Rep., 1996

Some other Issues!

- At low temperatures we see that most of the information is near $\tau = 0$ and $\tau = 0$ and $\tau = \beta$...this means that we will have very few points with the real information!

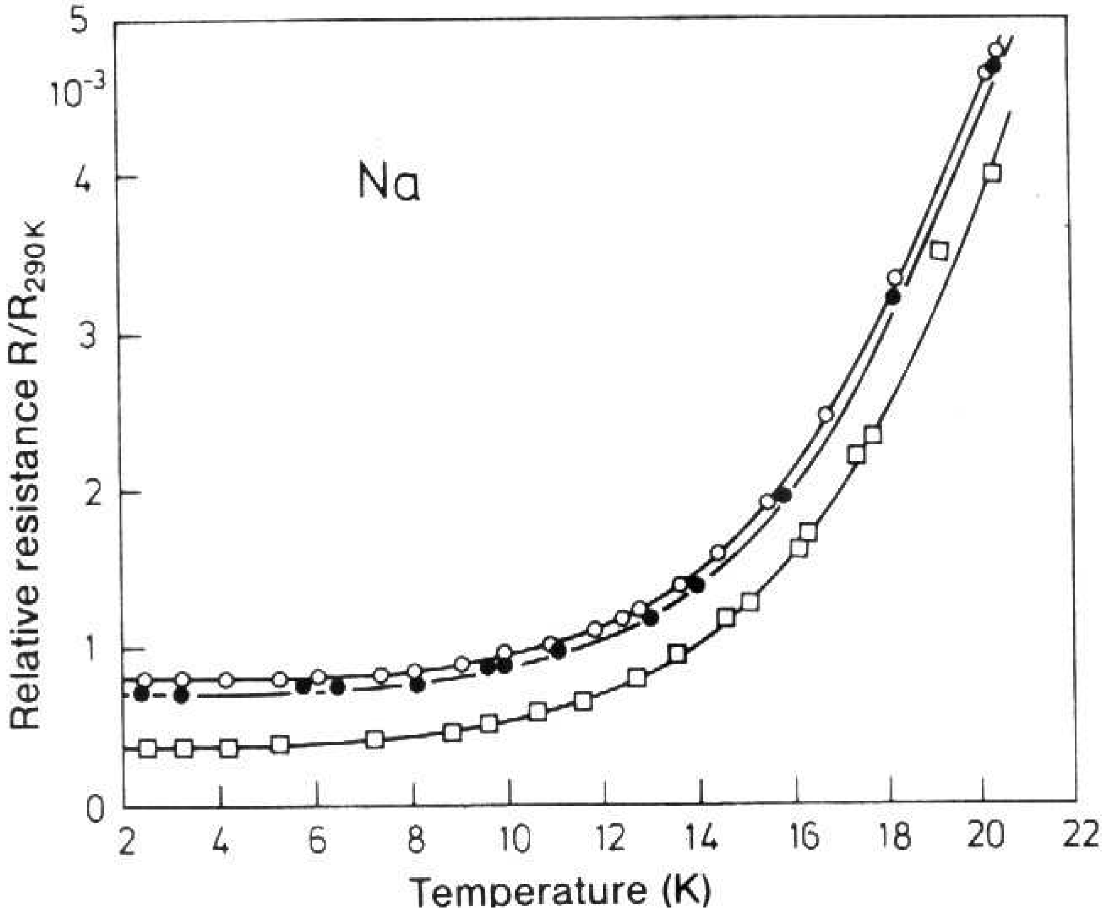


- Recent development to tackle this: Werner, Mills et al., PRL, 2006, "Continuous time Monte Carlo", evaluate certain class of perturbative diagrams using Monte Carlo

Numerical Renormalization Group

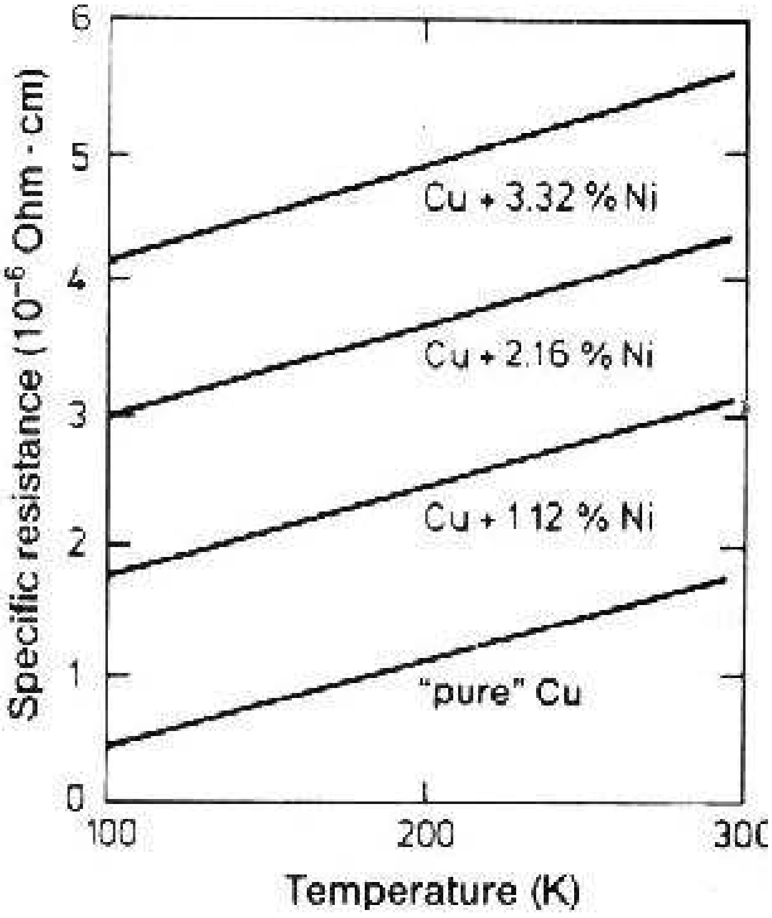
- **We will now get a flavour of what NRG is...**
- **Plan**
  - **To** *motivate* **this method, we will quickly review the Kondo effect, NRG was invented by Wilson (Nobel Prize 1982) to sort out the Kondo effect – the first** *non-perturbative* **application of RG ideas!**
  - **Poor Man's renormalization group idea of the Kondo problem**
  - **Wilson NRG**

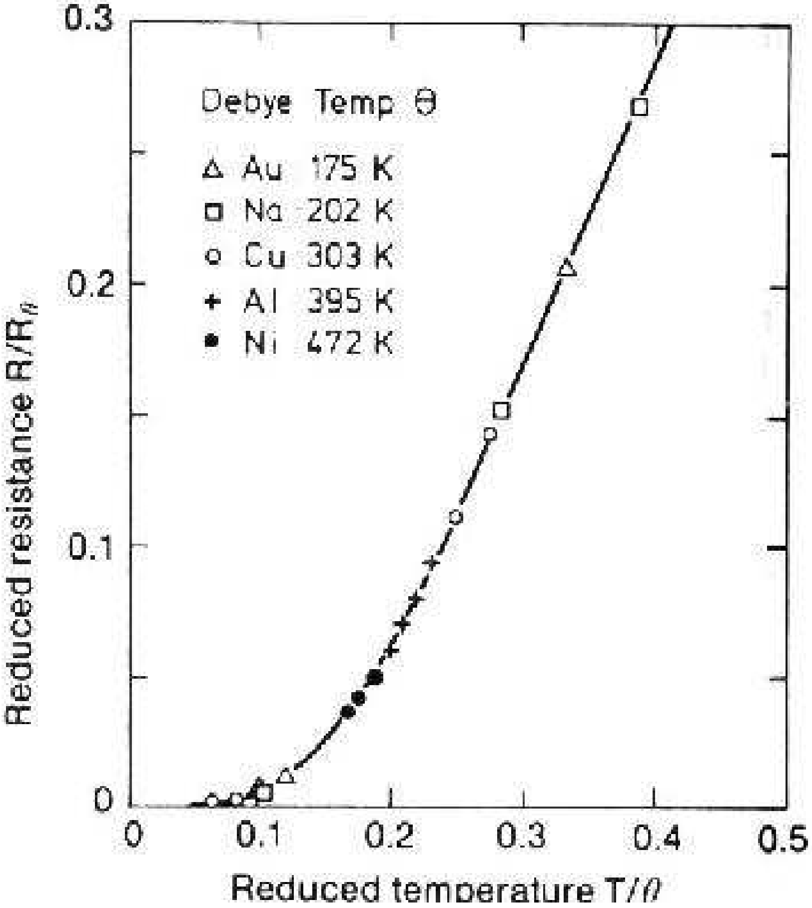
Resistivity in Metals



- **Almost constant at "low" temperatures...all way to linear at high temperatures**

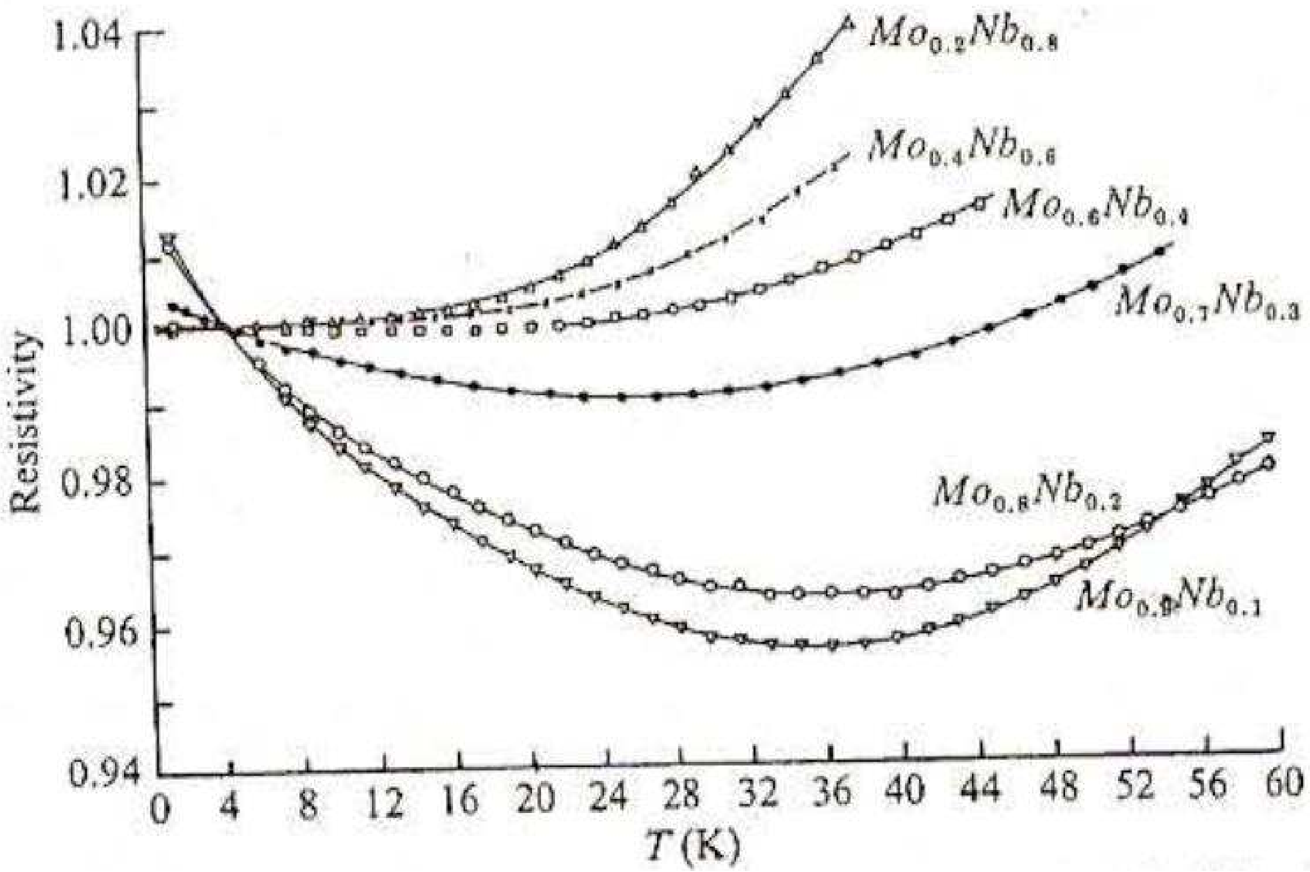
Resistivity in Metals...There's More!





- **Increases with impurity content**
- **Has some "universal" features...**

The Kondo Effect!



- **There is a “resistance minimum” in some cases!**

The sd Hamiltonian

- **The Hamiltonian**

$$H = \sum_{k\sigma} \varepsilon(k) c^\dagger_{k\sigma} c_{k\sigma} + J \boldsymbol{s} \cdot \boldsymbol{S}$$

$\boldsymbol{s} = \frac{1}{N} \sum_{k\sigma,k'\sigma'} c^\dagger_{k\sigma} \vec{\tau}_{\sigma\sigma'} c_{k'\sigma'}$ is the conduction electron spin at the impurity site (N is number of sites); J is an exchange term...

$$\frac{J}{2N} \sum_{k,k'} \left[\left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) S_z + c^\dagger_{k\uparrow} c_{k'\downarrow} S_- + c^\dagger_{k\downarrow} c_{k'\uparrow} S_+ \right]$$

Notice the spin flip scattering terms...

Poor Man's Approach to the Kondo Problem

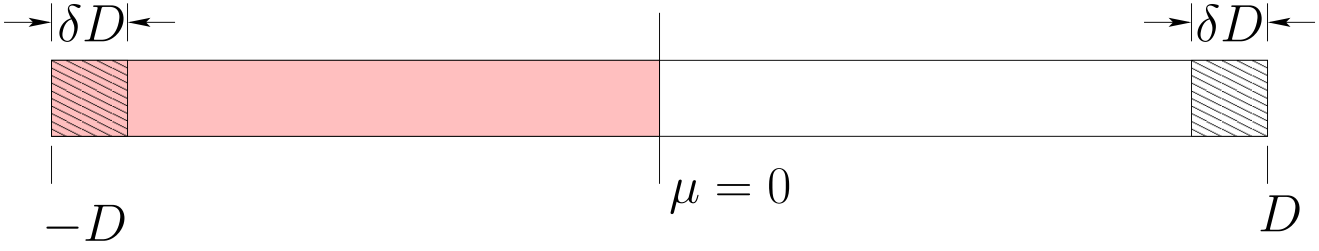
- Anderson asked the following question: What are the most important degrees of freedom in the Kondo problem? Can one write out an effective Hamiltonian just for these degrees of freedom?
- Clearly the key degrees of freedom at low temperatures are the states near the chemical potential... They can undergo scattering from the impurity that may be direct or spin-flip...
- He considered the Hamiltonian of the form

$$\sum_{k} \varepsilon(k) c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{k,k'} J_z \left(c^{\dagger}_{k\uparrow} c_{k'\uparrow} - c^{\dagger}_{k\downarrow} c_{k'\downarrow} \right) S_z + J_{\perp} c^{\dagger}_{k\uparrow} c_{k'\downarrow} S_{-} + J_{\perp} c^{\dagger}_{k\downarrow} c_{k'\uparrow} S_{+}$$

This is an "anisotropic sd Hamiltonain" with J_z, $J_{\perp}$...

Poor Man's Approach to the Kondo Problem

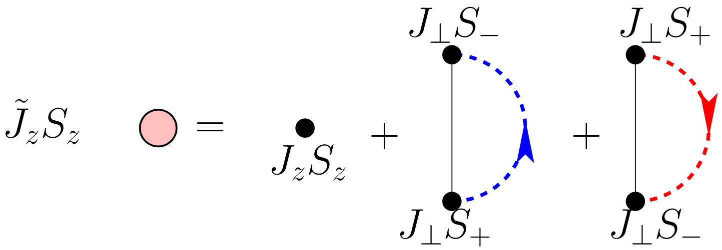
- **What is the** *effective Hamiltonian* **in the band reduced by** δD **as shown?**



- **We expect to get a Hamiltonian with the** *same form* **as the** *sd* **but with** *new* **"renormalized" values of the** J**s...**
- **How can we find the new** J**s? Let us say that** J_z **goes to** $\tilde{J}_z$**.... Interpret** J_z**: it is the amplitude for scattering from** $|k\uparrow\rangle$ **to** $|k'\uparrow\rangle$**...**
- **Now if** k, k' **belong to the reduced band, the amplitude of this scatteringy will be a sum of direct scattering in the band (**J_z**), and scattering from** k **to** k' **via all intermediate states which lie in the** *shaded part of the band* **(call this** δJ_z**)...**
- **Clearly we need only to worry about spin flip scattering..**

Poor Man's Approach to the Kondo Problem

- **Flow equation for Js best seen by diagrams**



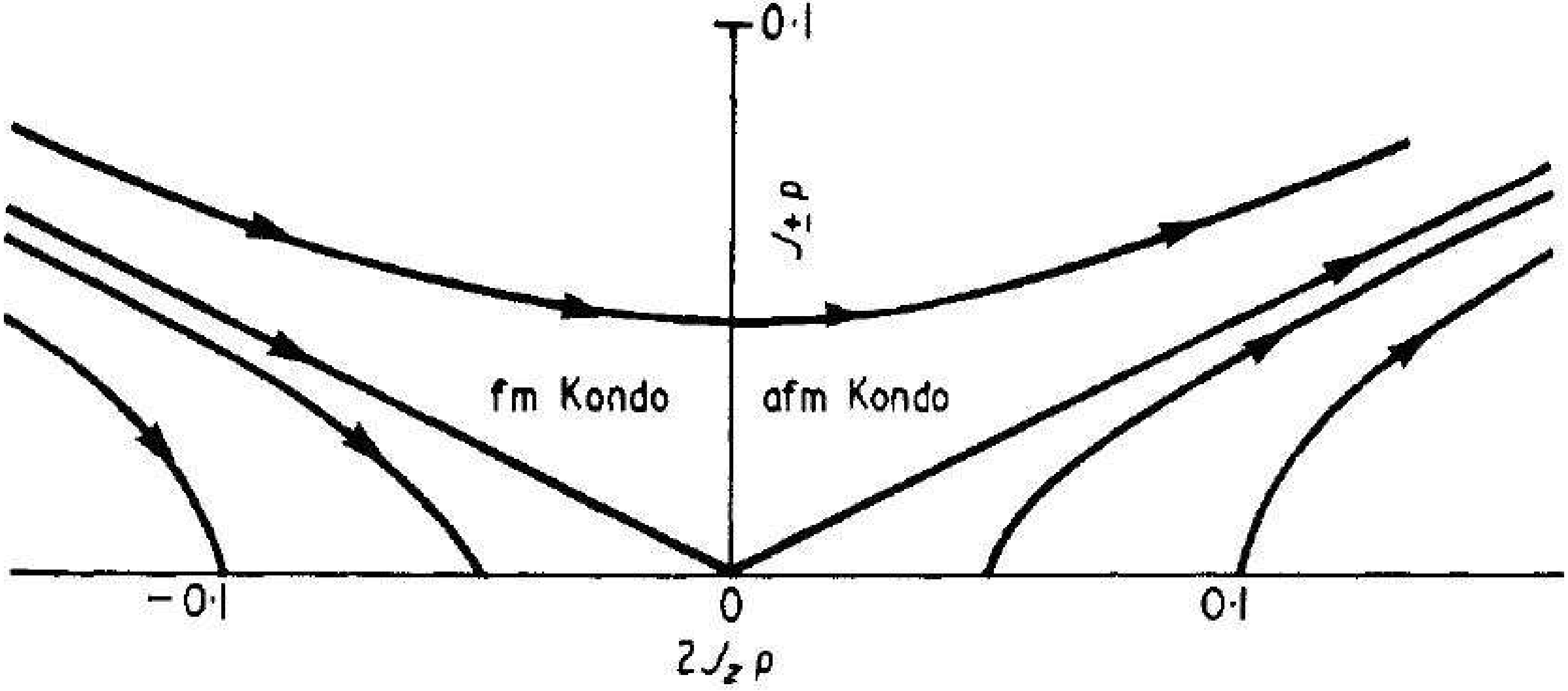
$$\delta J = J_\perp^2 S_- S_+ \left(-\rho_0 \frac{\delta D}{D}\right) + J_\perp^2 S_+ S_- \left(\rho_0 \frac{\delta D}{D}\right) = -2\rho_0 J_\perp^2 \left(\frac{\delta D}{D}\right) \Longrightarrow \frac{\mathrm{d} J_z}{\mathrm{d}\ln D} = -2\rho_0 J_\perp^2$$

- **With a similar equation for $J_\perp$, we have**

$$\begin{aligned} \frac{\mathrm{d} J_z}{\mathrm{d}\ln D} &= -2\rho_0 J_\perp^2 \\ \frac{\mathrm{d} J_\perp}{\mathrm{d}\ln D} &= -2\rho_0 J_\perp J_z \end{aligned}$$

Poor Man's Approach to the Kondo Problem

- **The solution $J_z^2 - J_\perp^2 = C$!**



- **Key point: Suppose we start with $J_z = J_\perp = J > 0$ (antiferromagnetic), then the coupling constant J flows to infinity...cannot do any pertubation theory**

Poor Man's Approach to the Kondo Problem

- **Note that for our sd-model, $De^{-\frac{1}{2J\rho_0}} = \bar{D}e^{-\frac{1}{2\bar{J}\rho_0}}$!! Thus the Kondo temperature is preserved along the trajectory!! Thus the key energy scale remains "invariant"**
- **Changing D is like changing T, and hence we expect all properties to be "universal functions" of $\frac{T}{T_K}$**
- **In many ways, this *is* the solution of the Kondo problem! But the full solution by Wilson is a treat in itself...**

Wilson's RG Appoach to Kondo Problem

- **Key observation: The problems are caused by a logarithmic divergence...consider** $\int_a^b \frac{\mathrm{d}\varepsilon}{\varepsilon} = \ln\left(\frac{b}{a}\right)$
- **We ask "why" is** $\int_0^1 \frac{\mathrm{d}\varepsilon}{\varepsilon} = \infty$**? To see this, break up** $[0,1]$ **into intervals** $[\Lambda^{-(n+1)}, \Lambda^{-n}]$ **with** $\Lambda > 1$**...Thus**

$$[0,1] = \bigcup_{n=0}^{\infty} [\Lambda^{-(n+1)}, \Lambda^{-n}] \quad \Longrightarrow \quad \int_0^1 \frac{\mathrm{d}\varepsilon}{\varepsilon} = \sum_{n=0}^{\infty} \int_{\Lambda^{-(n+1)}}^{\Lambda^{-n}} \frac{\mathrm{d}\varepsilon}{\varepsilon} = \sum_{n=0}^{\infty} \ln\Lambda = \infty!!$$

The divergence occurs because all the "logarithmic intervals" contribute *equally*...

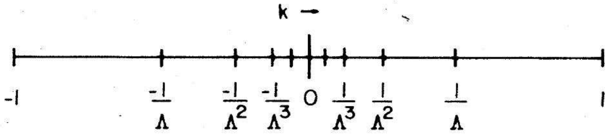
- **To study the Kondo model, Wilson considered a simplified Hamiltonian**

$$H = \int_{-1}^{1} \mathrm{d}k \, k c_{k\sigma}^{\dagger} c_{k\sigma} + J \boldsymbol{s} \cdot \boldsymbol{S}$$

Repeated σ **are summed here and henceforth**

Wilson's RG Appoach to The Kondo Problem

- **Starting from $H = \int_{-1}^{1} \mathrm{d}k \; k c^\dagger_{k\sigma} c_{k\sigma} + J \boldsymbol{s} \cdot \boldsymbol{S}$, and using log descretization**



reduced to

$$H = \frac{1}{2}(1+\Lambda^{-1}) \sum_{n=0}^{\infty} \Lambda^{-n} (c^\dagger_{+n\sigma} c_{+n\sigma} - c^\dagger_{-n\sigma} c_{-n\sigma}) + J \boldsymbol{s} \cdot \boldsymbol{S}$$

$c_{\pm n\sigma}$ **are electron operators to the right (left) of $\mu(k=0)$**

- **Now**

$$\boldsymbol{s} = \frac{1}{2} f^\dagger_{0\sigma} \vec{\tau}_{\sigma\sigma'} f_{0\sigma'} \qquad f_{0\sigma} = \frac{1}{\sqrt{2}} \int_{-1}^{1} \mathrm{d}k \; c_{k\sigma}$$

$$f_{0\sigma} \approx \left(\frac{1}{2}(1-\Lambda^{-1}) \right)^{1/2} \sum_{n=0}^{\infty} \Lambda^{-n/2} (c_{+n\sigma} + c_{-n\sigma})$$

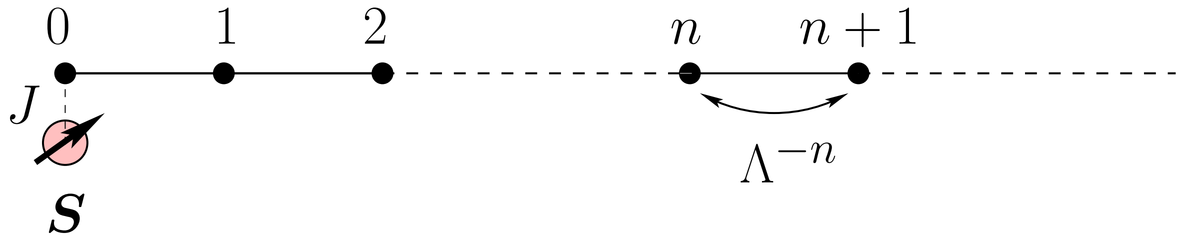
Thus, the impurity couples equally to states of *all energies*! This *is* the problem!

Wilson's RG Appoach to The Kondo Problem

- By sheer genius (bordering on subterfuge!) Wilson mapped this Hamiltonian to

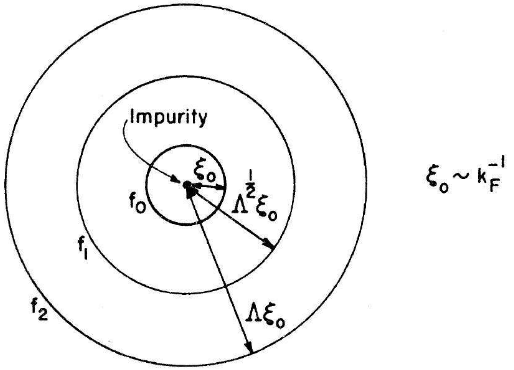
$$H = \sum_{n=0}^{\infty} \Lambda^{-n} (f^\dagger_{n\sigma} f^\dagger_{n+1\sigma} + f^\dagger_{n+1\sigma} f_{n\sigma}) + J \frac{1}{2} f^\dagger_{0\sigma} \vec{\tau}_{\sigma\sigma'} f_{0\sigma'} \cdot \boldsymbol{S}$$

- This is a "1-D" semi-infinite chain with the first site interacting with the impurity, and an exponentially falling hopping between neighbours!



- We know what $f^\dagger_{0\sigma}$ does...what do the operators $f^\dagger_{n\sigma}$ do?

Wilson's RG Appoach to The Kondo Problem



- $f^\dagger_{0\sigma}$ **corresponds to a "spherical wave packet" localized around the impuritiy...**$f^\dagger_{1\sigma}$ **is a wave packet which peaks at a larger distance from the impurity... and so on!**
- **Electrons can "hop" from one wavepacket state to the "neighbouring" wave packet states...**
- **The states** $f^\dagger_{n\sigma}$ **can be obtained from** $c^\dagger_{\pm n\sigma}$**...via Lanczos tridiagonalization of the kinetic energy!**
- **Why all this? Impurity now couples only to** *one state***!**

Wilson's RG Appoach to The Kondo Problem

- **Wilson then used a numerical renormalization group technique to diagnolize the Hamiltonian which involves the following step**
- **Define**

$$H_N = \Lambda^{(N-1)/2}\left(\sum_{n=0}^{N-1}\Lambda^{-n}(f^\dagger_{n\sigma}f^\dagger_{n+1\sigma} + f^\dagger_{n+1\sigma}f_{n\sigma}) + J\frac{1}{2}f^\dagger_{0\sigma}\vec{\tau}_{\sigma\sigma'}f_{0\sigma'}\cdot\boldsymbol{S}\right)$$

- **Why do this?: $N \to \infty$ is like taking $T \to 0$, note that $\Lambda^{(N-1)/2}J$ which is the effective exchange coupling at N (temperature T) goes to infinity as $N \to \infty$ $(T \to 0)$....**
- **Define a transformation** $H_{N+1} = \Lambda^{1/2}H_N + f^\dagger_{N\sigma}f_{N+1\sigma} + f^\dagger_{N+1\sigma}f_{N\sigma}$

Wilson's RG Appoach to The Kondo Problem

- **Take $J = 0$ to start with, and ask what happens for large N?**
- **You will see with a bit of thought that you will get two types of spectrum depending on if N is even or odd..**
- **For $\Lambda = 2$ Wilson showed that the eigenvalues are**

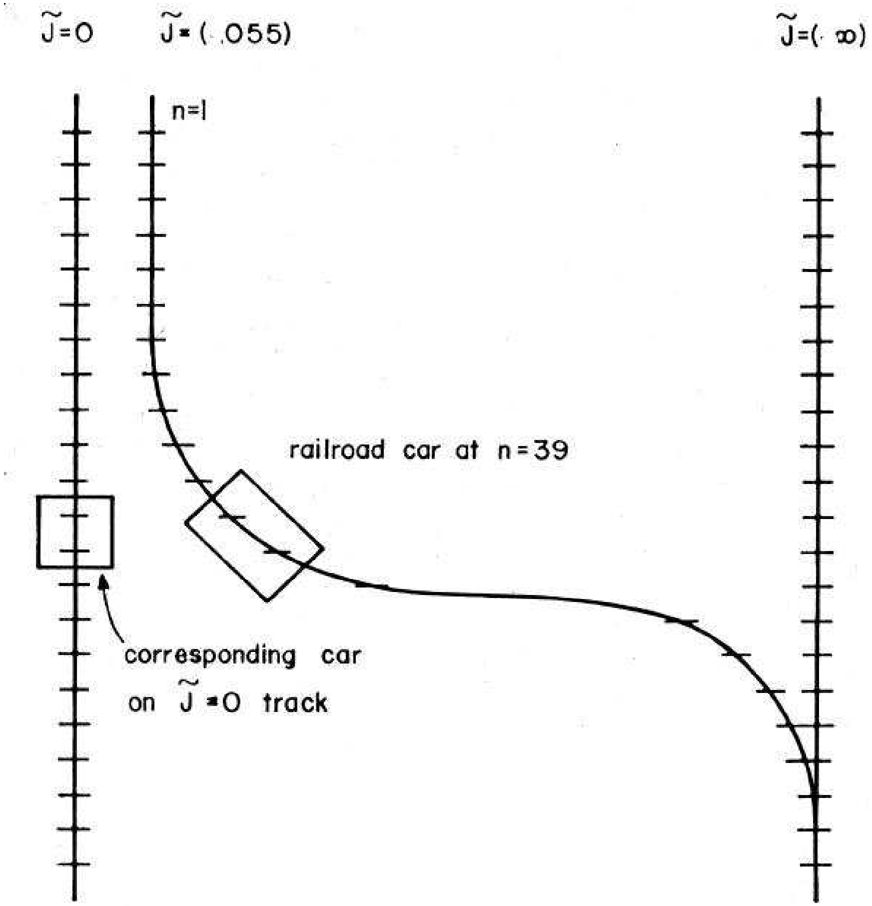
$$\begin{array}{rcl} \text{even } N & : & 0, \pm 1.297, \pm 2.827, \pm 4\sqrt{2} ... \pm 2^{\ell-1}\sqrt{2} .... \\ \text{odd } N & : & \pm 0.6555, \pm 1.976, \pm 4, \pm 8, ..., \pm 2^{\ell} \end{array}$$

- **Thus RG transformation $H_{N+2} = R[H_N]$ has two "fixed points" – one corresponding to even number N and another odd number N...**

Wilson's RG Appoach to The Kondo Problem

- **Now start with a very small $J \neq 0$...and focus on N even...**
- **Until N becomes large enough so that $J_{eff} = \Lambda^{(N-1)/2} J \leq 1$, the eigenvalues will look like those of even N...**
- **For even larger N the $J_{eff} \to \infty$...what does this mean...the site 0 will from a singlet with the impurity and completely drop out of the Hamiltonian...i. e., the site 0 will** *decouple* **from the chain since it fully couples with the impurity!!** *This means although there are N is even, the spectrum of H_N will be similar to that of odd N!*
- **When you start with a tiny J, there is a range of N (high T) where the behaviour is same as that of the $J = 0$ fixed point (this is where perturbation theory works)... and as N is increased it** *flows* **to the $J \to \infty$ fixed point (the Kondo singlet)!**
- **$J = 0$ is an** *unstable* **fixed point, $J = \infty$ is a stable fixed point...Best visualized by lifting a figure straight out of Wilson's** *RMP*

Wilson's RG Appoach to The Kondo Problem

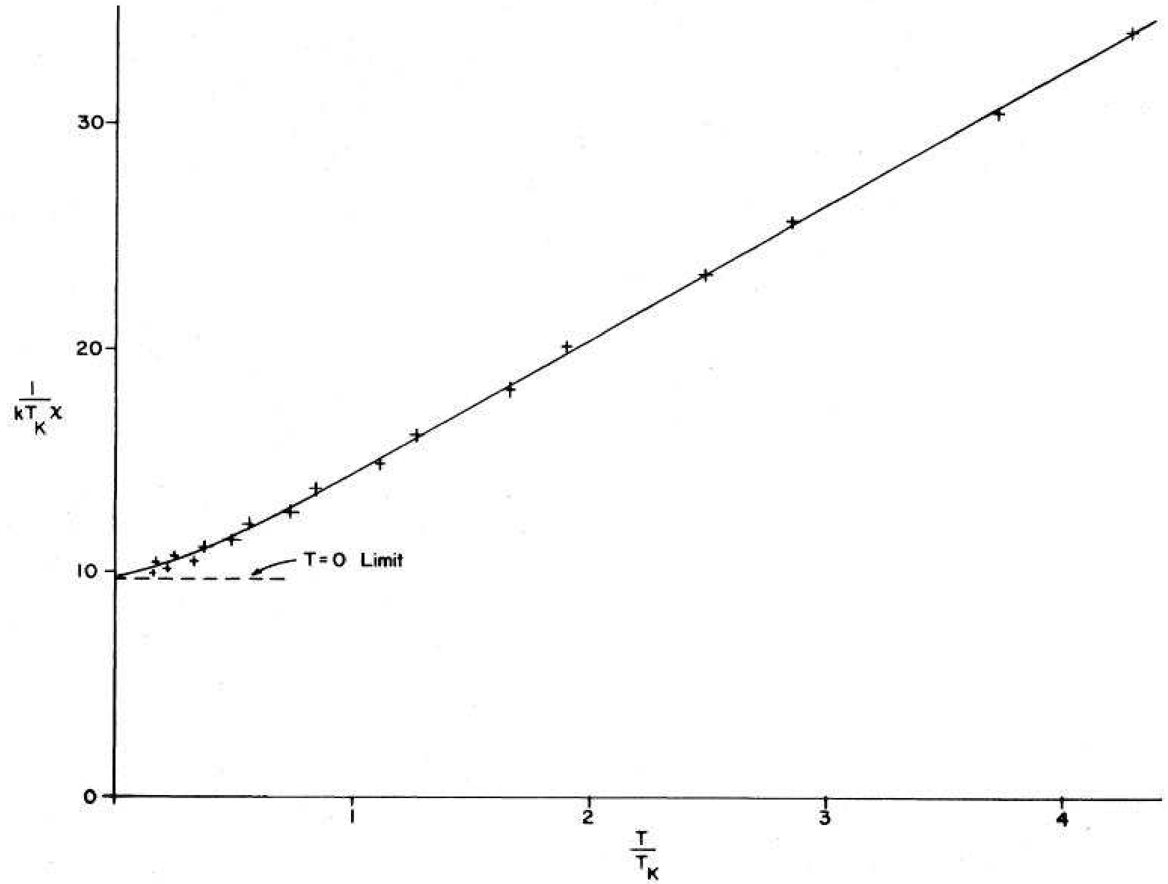


N	20	22	108	110	130	180
E_1	0.0314	0.0321	0.313	0.363	0.6541	0.6555
E_2	0.0419	0.0428	0.446	0.529	1.3055	1.3110

- **RG flow in the Kondo problem...all well and good..what about quantitative things?**

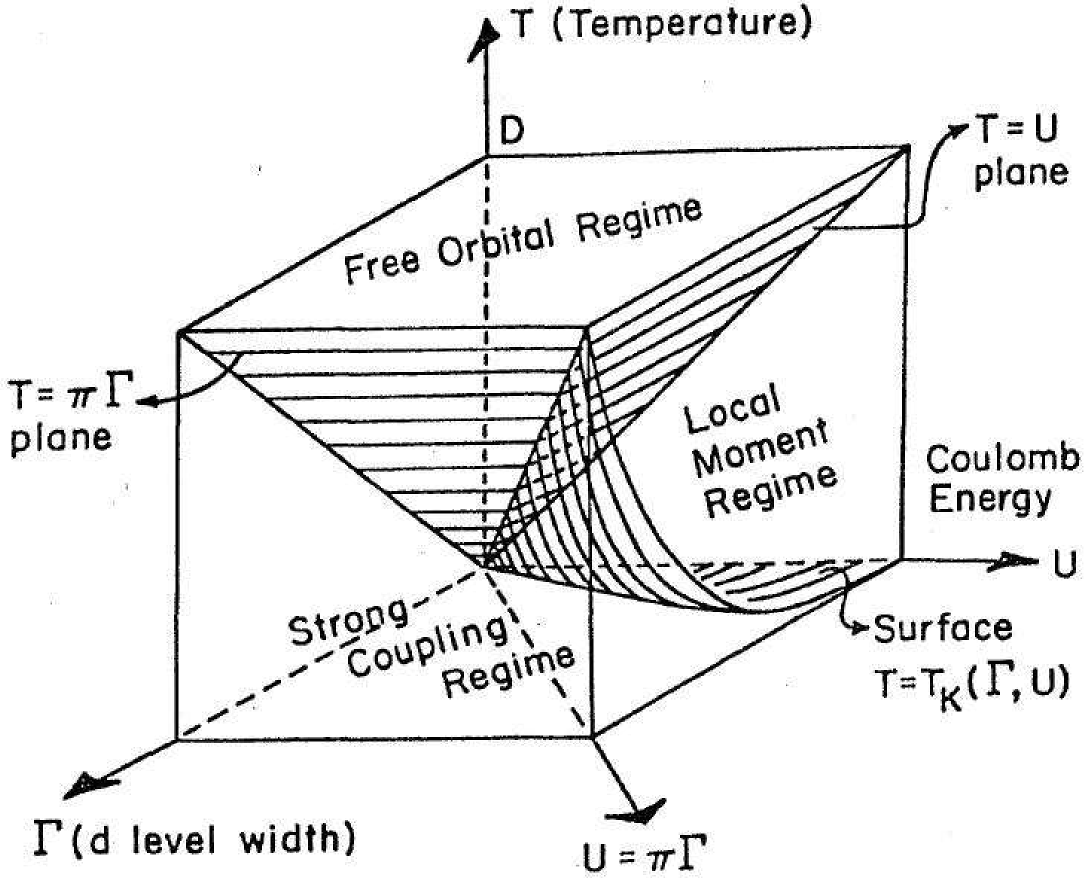
Wilson’s RG Appoach to The Kondo Problem

- **Using the fact that $T \sim \Lambda^{-N}$, and using an iterative scheme that correctly calculates the** *$low\ energy$* **excitations of the Hamiltonians at large N, Wilson obtained the universal function for susceptibility...**



What about the Anderson Model?

- **The Anderson model was solved by NRG techniques by Krishnamurthy et al.**



NRG and DMFT

- **Given $\mathcal{G}$, there are following steps that we need to implement DMFT**
  - **Need to get the "1-d" "tridiagonal" chain...this is a numerically tricky part and requires high precision numerics**
  - **Iterative diagonalization**
  - **Looking at states, matrix elements, etc., we can get $A(\omega)$...at least this is easy to say!**
- **The actual implementation is quite involved...talk to Nandan!**