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 Hamiltonians – simple to write down, hard to solve

Reason: Strong correlations, large couplings...

...

The “simple” Hubbard (“truncated” PPP) model

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

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

\[ G(k\sigma, \tau) = \langle T_{\tau} c_{k\sigma}(\tau) c_{k\sigma}^{\dagger}(0) \rangle \]

\( \tau \) is the imaginary time

- We can write this in the frequency domain as

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

- Analytic continuation of \( G(k\sigma, i\omega_n) \) from the upper \( \omega \) planes gives us

\[ G(k\sigma, i\omega_n) \implies \text{Analytical Continuation} \implies G^R(k\sigma, \omega^+) \]

the retarded Green's function
What are we looking for?

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

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

- This is an experimentally observable quantity

Undoped Bi2212, Damascelli et al. 2003
Some more elementary ideas

- The “bare Greens function”, $G$ for $U = 0$

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

$\varepsilon(k)$ – electronic dispersion

- The Dyson equation

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

$\Sigma(k\sigma, i\omega_n)$ is the “self energy”
Some more elementary ideas

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

$$ G_{i\sigma}(\tau) = \langle T_\tau c_{i\sigma}(\tau) c_{i\sigma}^\dagger(0) \rangle $$

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

$$ G_{i\sigma}(i\omega_n) = \frac{1}{N} \sum_k G(k\sigma, i\omega_n) $$

$$ = \frac{1}{N} \sum_k \frac{1}{i\omega_n - \varepsilon(k) + \mu - \Sigma(k\sigma, i\omega_n)} $$

$N$ - number of sites
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 $\alpha$ – 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...

$$H_A = \sum_\alpha \epsilon_\alpha b_{\alpha \sigma}^\dagger b_{\alpha \sigma} + U n_\uparrow n_\downarrow - \mu c_{\sigma}^\dagger c_{\sigma} + \sum_\alpha \gamma_\alpha (b_{\alpha \sigma}^\dagger c_{\sigma} + c_{\sigma}^\dagger b_{\alpha \sigma})$$

- **Bath**
- **Impurity**
- **Hybridization**

$b$s are the bath states, $\epsilon_\alpha$ and $\gamma_\alpha$, and even $\alpha$'s themselves are unknowns 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... $\epsilon_\alpha, \gamma_\alpha$!
Assume that we somehow know $\epsilon_\alpha$ and $\gamma_\alpha$

Suppose $U$ were zero, then we can solve the problem exactly (quadratic Hamiltonian!), and obtain the Green’s function of the impurity $G_\sigma(i\omega_n)$

Note that $G_\sigma(i\omega_n)$ has all the required information regarding $\epsilon_\alpha$ and $\gamma_\alpha$...i.e., this is what we take that we know

Key question: Suppose $G_\sigma(i\omega_n)$ 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 $G_\sigma(i\omega_n)$, 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 \[ \Sigma(k\sigma, i\omega_n) = \Sigma_\sigma(i\omega_n)! \]
  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

\[
G_{i\sigma}(i\omega_n) = \frac{1}{N} \sum_k \frac{1}{i\omega_n - \varepsilon(k) + \mu - \Sigma_\sigma(i\omega_n)}
\]

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 interactions” from $G_{i\sigma}(i\omega_n)$, i.e., what is

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

- This must be “mixing” with the rest of the lattice, i.e.,

$$G_{i\sigma}^{-1}(i\omega_n) + \Sigma_\sigma(i\omega_n) = G_\sigma(i\omega_n)$$

- Thus we get information about the bath! Note that everything on the LHS is determined by the bath which is specified by $G_\sigma$, and therefore the above equation is the self consistency equation!
We can now develop an iterative scheme to solve the self consistency equation...

Lattice Green’s Function
\[ G_i(i\omega_n) = \frac{1}{N} \sum_k \frac{1}{i\omega_n - (\epsilon(k) - \mu) - \Sigma(i\omega_n)} \]

Self Consistency
\[ G'_i(i\omega_n) = G_i(i\omega_n) + \Sigma(i\omega_n) \]

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)

Monte Carlo Method for Magnetic Impurities in Metals

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and

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(Received 17 March 1986)

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:** $G_\sigma(\tau)$, **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

$$\mathcal{H} = \left( \frac{U}{2} - \mu \right) (n_\uparrow + n_\downarrow) + \sum_{j=2}^{M} \varepsilon_j c_j^{\dagger} c_j \sigma + \sum_{j=2}^{M} \gamma_j \left( c_j^{\dagger} c_\sigma + c_\sigma^{\dagger} c_j \sigma \right)$$

\[ \mathcal{H}_0 - \text{Noninteracting part} \]

\[ + U \left( n_\uparrow n_\downarrow - \frac{1}{2} (n_\uparrow + n_\downarrow) \right) \]

\[ \mathcal{U} - \text{Interacting part} \]

We have dropped $A$ subscript on the Hamiltonian, $c_\sigma$ with out a $j$ stands for the impurity i.e., $j = 1$ etc.

Notation for quadratic operators, we write $A = \sum_{i,j} A_{ij} c_{i\sigma}^{\dagger} c_{j\sigma}$ where $A$ is a matrix.
HF-QMC: Times Slices

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

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

- So far there is no approximation of any kind!
HF-QMC: Times Slices

$\tau = 0$  $s_1$

Bath site  Impurity  $M$ sites

$\tau = \beta$

$\Delta \tau$

$\tau$

$s_L$

$L$

$\ell$

1
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 \( \Delta \tau \to 0 \)...this is the only source of systematic error in this method

With this approximation

\[
Z = \text{Tr} \left( \prod_{\ell=1}^{L} e^{-\Delta \tau \mathcal{H}_0} e^{-\Delta \tau \mathcal{U}} \right)
\]
We now use the identity

\[ e^{-\Delta \tau U} = \frac{1}{2} \sum_{s=\pm 1} e^{\lambda_s(n_\uparrow - n_\downarrow)} \]

if \( \lambda \) 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 \( \lambda \) is chosen appropriately
Now take the term $e^{-\Delta \tau U}$ in the $\ell$-th time slice and use the HHS identity to get

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

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

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

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

$$e^{-\Delta \tau \mathcal{H}_0} e^{-\Delta \tau \mathcal{U}} \bigg|_\ell = \frac{1}{2} \sum_{s_\ell} e^{-\Delta \tau \mathcal{H}_{0\uparrow}} e^{\mathcal{V}_\uparrow(\ell)} e^{-\Delta \tau \mathcal{H}_{0\downarrow}} e^{\mathcal{V}_\downarrow(\ell)}$$
Now the partition function can be written as

\[ Z = \left( \frac{1}{2} \right)^L \sum_{\{s_1, \ldots, s_L\}} \text{Tr} \left( \prod_{\ell=1}^L e^{-\Delta \tau \mathcal{H}_0 \uparrow} e^{V_\uparrow (\ell)} e^{-\Delta \tau \mathcal{H}_0 \downarrow} e^{V_\downarrow (\ell)} \right) \]

This can be recast as \textbf{Question: Why?}

\[ Z = \left( \frac{1}{2} \right)^L \sum_{\{s_1, \ldots, s_L\}} \text{Tr} \left( \prod_{\ell=1}^L e^{-\Delta \tau \mathcal{H}_0 \uparrow} e^{V_\uparrow (\ell)} \right) \text{Tr} \left( \prod_{\ell=1}^L e^{-\Delta \tau \mathcal{H}_0 \downarrow} e^{V_\downarrow (\ell)} \right) \]

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

\[ Z = \sum_{\{s_1, \ldots, s_L\}} \text{some function of} \{s_1, \ldots, s_L\} \]

We have achieved our goal \textit{in principle}; we now evaluate the “some function”
**Lemma I:** Let $A = \sum_{ij} A_{ij} c_i^\dagger c_j$ Question: Why are there no spin indices?, then

$$\text{Tr} e^{-A} = \det (1 + e^{-A})$$

Proof is quite easy...

**Lemma II:** Consider quadratic operators $A, B, C..., $ then

$$\text{Tr}(e^{-A}e^{-B}e^{-C}...) = \det (1 + e^{-A}e^{-B}e^{-C}...)$$
HF-QMC: The Partition Function

With these lemmas, we can write

\[ Z = \sum_{\{s_1, \ldots, s_L\}} \det \left( 1 + e^{-\Delta \tau \mathcal{H}_0} e^{V_{\uparrow}(1)} \ldots e^{-\Delta \tau \mathcal{H}_0} e^{V_{\uparrow}(\ell)} \ldots e^{-\Delta \tau \mathcal{H}_0} e^{V_{\uparrow}(L)} \right) \times \]

\[ \det \left( 1 + e^{-\Delta \tau \mathcal{H}_0} e^{V_{\uparrow}(1)} \ldots e^{-\Delta \tau \mathcal{H}_0} e^{V_{\uparrow}(\ell)} \ldots e^{-\Delta \tau \mathcal{H}_0} e^{V_{\uparrow}(L)} \right) \]

Question: What has been dropped? Is it okay?

Now following the standard route, we define matrices

\[ \mathbb{B}_\sigma(\ell) = e^{-\Delta \tau \mathcal{H}_0 \sigma} e^{V_{\sigma}(\ell)} \]

to get

\[ Z = \sum_{\{s_1, \ldots, s_L\}} \det \left( 1 + \mathbb{B}_{\uparrow}(L) \ldots \mathbb{B}_{\uparrow}(\ell) \ldots \mathbb{B}_{\uparrow}(1) \right) \det \left( 1 + \mathbb{B}_{\downarrow}(L) \ldots \mathbb{B}_{\downarrow}(\ell) \ldots \mathbb{B}_{\downarrow}(1) \right) \]
Now with a little bit of matrix algebra one can show that

$$\det (1 + \mathbb{B}_\sigma(L) \ldots \mathbb{B}_\sigma(\ell) \ldots \mathbb{B}_\sigma(1)) = \det \varnothing_\sigma(\{s_\ell\})$$

where

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

which is an $L \times L$ matrix of $M \times M$ matrices
The partition function is now

\[ Z = \sum_{\{s_1, \ldots, s_L\}} \det \mathcal{O}_\uparrow(\{s_\ell\}) \det \mathcal{O}_\downarrow(\{s_\ell\}) \]

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

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

We can now interpret \( \det \mathcal{O}_\uparrow(\{s_\ell\}) \det \mathcal{O}_\downarrow(\{s_\ell\})/Z \) as the statistical weight of the Ising spin configuration!
HF-QMC: The Algorithm

This will be perfectly fine if \( \det \mathcal{O}_\uparrow(S) \det \mathcal{O}_\downarrow(S) \) 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 \( \{s_\ell\} \rightarrow \{s'_\ell\} \), you have to calculate

\[
r = \frac{\det \mathcal{O}_\uparrow(s'_\ell) \det \mathcal{O}_\downarrow(s'_\ell)}{\det \mathcal{O}_\uparrow(s_\ell) \det \mathcal{O}_\downarrow(s_\ell)}
\]
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 $G$

....

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 Observations

- What is the “meaning” of the matrix $O_\sigma(\{s_\ell\})$?

- A little thought will tell you that $G_\sigma(\{s_\ell\}) = O_\sigma^{-1}(\{s_\ell\})$, 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,

$$
(G_\sigma(\{s_\ell\}))(\ell_1, i);(\ell_2, j) = \langle c_i \sigma(\ell_1) c_j^\dagger \sigma(\ell_2) \rangle_{\{s_\ell\}}, \ \ell_1 > \ell_2
$$

- Specifically,

$$
(G_\sigma(\{s_\ell\}))_{\ell_1, \ell_2} = (G_\sigma(\{s_\ell\}))(\ell_{1, 1};(\ell_{2, 1}) = \langle c_\sigma(\ell_1) c_\sigma^\dagger(\ell_2) \rangle_{\{s_\ell\}}, \ \ell_1 > \ell_2
$$

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 $G_\sigma(\{s_\ell\})$. 
HF-QMC: Key Observations

- $G_\sigma(\{s_\ell\})$ 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 $G_\sigma(\{s'_\ell\}) = G'_\sigma$ satisfies a Dyson-like equation

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

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

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

- There is more...
HF-QMC: Key Observations

- Here is the punch line observation of Hirsch-Fye...
- The new impurity Green’s function matrix $G'_\sigma$ also satisfies a Dyson equation of the form

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

where $1$ is a $L \times L$ identity, and $V$ 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?

$$G_\sigma = G_\sigma + (G_\sigma - 1)e^{-V}G_\sigma$$
HF-QMC: Key Observations

Thus if we know $G$ (which we do!), we can calculate $G_\sigma$ which depends on the Ising spin configuration!

And, here is the final observation

\[
\frac{\det \mathcal{O}_\sigma'}{\det \mathcal{O}_\sigma} = \frac{\det G_\sigma}{\det G'_\sigma}
\]

Happily, now

- We need to worry only about $L \times L$ determinants!
- We need only $G$!

A couple of more technical things...
HF-QMC: Key Observations

- Note when we go from spin configuration $s$ to $s'$ we flip the spin only at one $\tau$-site, say $\ell$...

- It turns out that we can explicitly calculate the ratio of the determinants

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

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

- If the new configuration is accepted, then we have to update $G_{\sigma}$...there is an $L \times L$ efficient formula

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

- Input, the matrix $G$, choose $L$
- Generate a random string of Ising spins $\{s_\ell\}$; set up $G$
  using $G_\sigma = G_\sigma + (G_\sigma - 1)e^{-V}G_\sigma$
- 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
The Anderson impurity problem is specified by three parameters

1. $\varepsilon_d$ – $d$-orbital (impurity) energy level
2. $\Delta$ – effective hybridization parameter
3. $U$ – Coulomb repulsion

The bare Greens function $G$ can be explicitly calculated as

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

For the symmetric model $\varepsilon_d = -U/2$, the Kondo temperature is $T_K \sim \sqrt{\frac{\Delta}{U}} e^{-\frac{\pi U}{8\Delta}}$.
HF-QMC Example: Anderson Impurity Problem

• HFQMC code – freely available with this lectures
HF-QMC Example: Anderson Impurity Problem

System with $T_K = 0.03$

![Graph showing $G_\uparrow$ and $curly G_\uparrow$ versus $\tau/\beta$.](image)

- $U = 4.0$
- $\Delta = 0.5$
- $T_K = 0.03$
- $T = 0.5$
System with $T_K = 0.03$

$U=4.0$
$\Delta=0.5$
$T=0.05$

$G_{\uparrow}$ (QMC)

curly $G_{\uparrow}$
HF-QMC Example: Anderson Impurity Problem

System with $T_K = 0.03$

- $U = 4.0$
- $\Delta = 0.5$
- $T = 0.005$

$G$ vs $\tau/\beta$

$G_{\uparrow}$ (QMC)
HF-QMC Example: Anderson Impurity Problem

Susceptibility

\[ \chi \]

- \( U = 1.0 \)
- \( \Delta = 0.1 \)
- \( T_K \approx 0.01 \)

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 $G_\sigma$ can give very wild answers! Ill-posed!
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 $p_i$? Shannon’s solution: Maximize the information entropy $S[p] = -\sum_i p_i \ln p_i$

We maximize $S[p]$ subject to the known conditions
Back to our problem, we know $G_\sigma(\tau)$ for a discrete set of values

This is related to $A_\sigma(\omega)$ by

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

Also we know that $\int_{-\infty}^{\infty} d\omega A(\omega) = 1$

Information entropy $S[A] = -\int_{-\infty}^{\infty} d\omega A(\omega) \ln A(\omega)$

Maximize $S[A]$, with knowledge of the errors in the QMC (Gubernatis et al. 1991)
Maximum Entropy

Solution of the Anderson impurity problem

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

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

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

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

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

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

This is an “anisotropic $sd$ Hamiltonian” with $J_z$, $J_\perp$...
What is the effective Hamiltonian in the band reduced by $\delta D$ as shown?

![Diagram showing bands reduced by $\delta D$.]

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 scattering 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 $\delta J_z$)...

Clearly we need only to worry about spin flip scattering..
Poor Man’s Approach to the Kondo Problem

- Flow equation for \( J \)'s best seen by diagrams

\[
\tilde{J}_z S_z = J_z S_z + J_\perp S_+ + J_\perp S_-
\]

\[
\delta J = J_\perp S_- S_+ \left( -\rho_0 \frac{\delta D}{D} \right) + J_\perp S_+ S_- \left( \rho_0 \frac{\delta D}{D} \right) = -2\rho_0 J_\perp^2 \left( \frac{\delta D}{D} \right) \implies \frac{dJ_z}{d\ln D} = -2\rho_0 J_\perp^2
\]

- With a similar equation for \( J_\perp \), we have

\[
\frac{dJ_z}{d\ln D} = -2\rho_0 J_\perp^2
\]

\[
\frac{dJ_\perp}{d\ln D} = -2\rho_0 J_\perp J_z
\]
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 perturbation theory
Poor Man’s Approach to the Kondo Problem

- Note that for our $sd$-model, $D e^{-\frac{1}{2J\rho_0}} = \bar{D} e^{-\frac{1}{2J\rho_0}}$!! 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 \textit{is} the solution of the Kondo problem! But the full solution by Wilson is a treat in itself...
Wilson’s RG Approach to Kondo Problem

- Key observation: The problems are caused by a logarithmic divergence...consider  ∫_a^b \frac{d\varepsilon}{\varepsilon} = \ln \left( \frac{b}{a} \right)

- We ask “why” is ∫_0^1 \frac{d\varepsilon}{\varepsilon} = \infty? To see this, break up [0, 1] into intervals [\Lambda^{-(n+1)}, \Lambda^{-n}] with \Lambda > 1...Thus

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

The divergence occurs because all the “logarithmic intervals” contribute equally...

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

\[ H = \int_{-1}^{1} dk \; k c_{k\sigma}^\dagger c_{k\sigma} + J s \cdot S \]

Repeated \( \sigma \) are summed here and henceforth
Wilson’s RG Approach to The Kondo Problem

Starting from \( H = \int_{-1}^{1} dk \, k c_{k\sigma}^{\dagger} c_{k\sigma} + J s \cdot S \), and using log descretization

reduced to

\[
H = \frac{1}{2} \left( 1 + \Lambda^{-1} \right) \sum_{n=0}^{\infty} \Lambda^{-n} (c_{+n\sigma}^{\dagger} c_{+n\sigma} - c_{-n\sigma}^{\dagger} c_{-n\sigma}) + J s \cdot S
\]

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

Now

\[
s = \frac{1}{2} f_{0\sigma}^{\dagger} \tau_{\sigma\sigma'} f_{0\sigma'} \quad f_{0\sigma} = \frac{1}{\sqrt{2}} \int_{-1}^{1} dk \, c_{k\sigma}
\]

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

Thus, the impurity couples equally to states of all energies! This is the problem!
By sheer genius (bordering on subterfuge!) Wilson mapped this Hamiltonian to

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

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 $f_{0\sigma}^{\dagger}$ does...what do the operators $f_{n\sigma}^{\dagger}$ do?
Wilson’s RG Approach to The Kondo Problem

- $f_{0\sigma}^+$ corresponds to a “spherical wave packet” localized around the impurity... $f_{1\sigma}^+$ 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 $f_{n\sigma}^+$ can be obtained from $c_{\pm n\sigma}^+$... via Lanczos tridiagonalization of the kinetic energy!

- Why all this? Impurity now couples only to one state!
Wilson’s RG Approach to The Kondo Problem

Wilson then used a numerical renormalization group technique to diagonalize the Hamiltonian which involves the following step

Define

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

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

\[ H_{N+1} = \Lambda^{1/2} H_N + f_{N\sigma}^\dagger f_{N+1\sigma} + f_{N+1\sigma}^\dagger f_{N\sigma} \]
Wilson’s RG Approach 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
  
  $\begin{align*}
  \text{even } N & : \quad 0, \pm 1.297, \pm 2.827, \pm 4\sqrt{2}... \pm 2^{\ell-1}\sqrt{2}... \\
  \text{odd } N & : \quad \pm 0.6555, \pm 1.976, \pm 4, \pm 8,..., \pm 2^\ell
  \end{align*}$

- 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 Approach 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 $J_{\text{eff}} = \Lambda^{(N-1)/2} J \leq 1$, the eigenvalues will look like those of even $N$...

- For even larger $N$ the $J_{\text{eff}} \to \infty$...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 Approach to The Kondo Problem

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