The Fermi gas in Dynamic Mean Field Theory

Nir Barnea

The Hebrew University, Jerusalem, Israel
INT, U. Washington, Seattle, WA

October, 2007
Introduction

Dynamic Mean Field Theory (DMFT)
An exact method for strongly correlated lattice fermions in infinite dimensions.

Georges and Kotliar, PRB 45, 6479 (1992)
## Introduction

**Dynamic Mean Field Theory (DMFT)**

An exact method for strongly correlated lattice fermions in infinite dimensions.

Georges and Kotliar, PRB 45, 6479 (1992)

---

### Having Nuclear Physics in Mind

- Fermi Gas with contact interaction - A limiting case of neutron matter.
- Experimentally accessible using cold atoms.
- Perfect “playground” for many-body theories.
Outline

1 **DMFT**
   - Lattice Fermions in $d = \infty$ Dimensions
   - The Mean Field Theory
   - Solving the Impurity Model

2 **Fermi Gas with Contact Interaction**
   - Discretization
   - Scattering Length and Effective Range

3 **Extracting the Physics**

4 **Results**
Lattice Fermions in $d = \infty$ Dimensions

Consider the Hubbard model in $d$-dimensions

$$
\mathcal{H} = \sum_{ij\sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + \frac{1}{2} U \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} c_{i,-\sigma}^\dagger c_{i,-\sigma}
$$

For a simple cubic lattice

$$
\epsilon_k = t_0 (2d - 2 \sum_{j=1}^{d} \cos k_j) \quad ; \quad t_0 = \frac{\hbar^2}{2ma^2}
$$

where $k_j = (\frac{2\pi}{N} \cdot \text{integer})$ for a box of size $(Na)^d$.

For $d \rightarrow \infty$ the hopping $t_0$ should be scaled as $1/\sqrt{d}$ to yield a nontrivial model.
Lattice Fermions in $d = \infty$ Dimensions

Consider the Hubbard model in $d$-dimensions

$$
\mathcal{H} = \sum_{ij\sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + \frac{1}{2} U \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} c_{i,\sigma}^\dagger c_{i,-\sigma} c_{i,-\sigma}
$$

For a simple cubic lattice

$$
\epsilon_k = t_0 (2d - 2 \sum_{j=1}^{d} \cos k_j) \quad ; \quad t_0 = \frac{\hbar^2}{2ma^2}
$$

where $k_j = (\frac{2\pi}{N} \cdot \text{integer})$ for a box of size $(Na)^d$.

For $d \rightarrow \infty$ the hopping $t_0$ should be scaled as $1/\sqrt{d}$ to yield a nontrivial model.

At this limit

$$
\delta(k) = \frac{1}{N^d} \sum_{n \in \text{sites}} e^{i \frac{2\pi}{N} n \cdot k} \rightarrow 1
$$

Consequently the self-energy becomes a local function.

W. Metzner and D. Vollhardt, PRL 62, 324 (1989)
The Green’s function and Self-Energy

- By definition the Green’s function is given by
  \[ G_{ij,\sigma}(\tau - \tau') \equiv \langle T c_{i,\sigma}(\tau) c_{j,\sigma}^\dagger(\tau') \rangle \]

- The Green’s function and the Self-energy are related through
  \[ G_{\sigma}(k, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma}(k, i\omega_n)} ; \quad \omega_n \equiv \frac{(2n + 1)\pi}{\beta} \]
The Green’s function and Self-Energy

- By definition the Green’s function is given by

\[ G_{ij,\sigma}(\tau - \tau') \equiv \langle T c_{i,\sigma}(\tau) c_{j,\sigma}^\dagger(\tau') \rangle \]

- The Green’s function and the Self-energy are related through

\[ G_{\sigma}(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\sigma}(\mathbf{k}, i\omega_n)} \quad ; \quad \omega_n \equiv \frac{(2n + 1)\pi}{\beta} \]

At the limit \( d \rightarrow \infty \)

Momentum space

\[ \Sigma_{\sigma}(\mathbf{k}, i\omega_n) \longrightarrow \Sigma_{\sigma}(i\omega_n) \]

The Fourier transform of the Green’s function takes a simple dependence on \( \mathbf{k} \),

\[ G_{\sigma}(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\sigma}(i\omega_n)} \]

Coordinate space

\[ \Sigma_{ij,\sigma}(i\omega_n) \longrightarrow \delta_{ij} \Sigma_{\sigma}(i\omega_n) \]

The site-diagonal Green’s function

\[ G_{ii,\sigma}(i\omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\sigma}(i\omega_n)} \]
Consider the effective action

\[ S_{\text{eff}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{i,\sigma}^\dagger(\tau) G_0^{-1}(\tau - \tau') c_{i,\sigma}(\tau') \]
\[ + U \int_0^\beta d\tau \, n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) \]
Consider the effective action

\[
S_{\text{eff}} = -\int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \sum_{\sigma} c_{i,\sigma}^\dagger(\tau) G_0^{-1}(\tau - \tau') c_{i,\sigma}(\tau') + U \int_{0}^{\beta} d\tau n_{i\uparrow}(\tau) n_{i\downarrow}(\tau)
\]  

The corresponding Green's function is given by

\[
\mathcal{G}(\tau - \tau') = \langle T c_{i,\sigma} c_{i,\sigma}^\dagger \rangle S_{\text{eff}}
\]  

The connection to the physical lattice is made through the demand

\[
G(\tau - \tau') = G_{ii}(\tau - \tau').
\]
The single-site impurity model

Consider the effective action

\[ S_{\text{eff}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{i,\sigma}^\dagger(\tau) G_0^{-1}(\tau - \tau') c_{i,\sigma}(\tau') + U \int_0^\beta d\tau \, n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) \]  

(1)

The corresponding Green’s function is given by

\[ G(\tau - \tau') = \langle T c_{i,\sigma} c_{i,\sigma}^\dagger \rangle S_{\text{eff}} \]  

(2)

and the self-energy is defined from the interacting Green’s function

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

(3)
The single-site impurity model

Consider the effective action

\[
S_{\text{eff}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{i,\sigma}^\dagger(\tau) G_0^{-1}(\tau - \tau') c_{i,\sigma}(\tau') + U \int_0^\beta d\tau \, n_{i\uparrow}(\tau) n_{i\downarrow}(\tau)
\]  

(1)

The corresponding Green’s function is given by and the self-energy is defined from the interacting Green’s function

\[
G(\tau - \tau') = \langle T c_{i,\sigma} c_{i,\sigma}^\dagger \rangle S_{\text{eff}} \quad \text{(2)}
\]

\[
\Sigma(i\omega_n) = G_0^{-1}(i\omega_n) - G^{-1}(i\omega_n) \quad \text{(3)}
\]

The connection to the physical lattice is made through the demand

\[
G(\tau - \tau') = G_{ii}(\tau - \tau') \quad \text{(4)}
\]
DMFT - The self-consistency condition

\[ S_{eff}[G_0] \]
The self-consistency condition

\[ S_{\text{eff}}[G_0] \]

\[ G, \Sigma = G_0^{-1} - G^{-1} \]
DMFT - The self-consistency condition

\[ S_{eff}[G_0] \]

\[ G, \Sigma = G_0^{-1} - G^{-1} \]

\[ G_{ii} = \sum \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma} \]
\[
S_{\text{eff}}[G_0]
\]

\[
G_0^{-1} = G_{ii}^{-1} + \Sigma
\]

\[
G_{ii} = \sum \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma}
\]

\[
G, \Sigma = G_0^{-1} - G^{-1}
\]
DMFT - The self-consistency condition

\[ S_{eff}[G_0] \]

\[ G_0^{-1} = G_{ii}^{-1} + \Sigma \]

\[ G_{ii} = \sum \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma} \]

\[ G, \Sigma = G_0^{-1} - G^{-1} \]
DMFT - General features

- Exact for $d \rightarrow \infty$

Free Fermi gas is recovered when the interaction is switched off.

At $U \rightarrow 0$ DMFT reproduces first order perturbation theory.

Gives the correct result in the atomic limit, $U \rightarrow \infty$.

The approximation $\Sigma(k, i\omega_n) \approx \Sigma(i\omega_n)$ can be relaxed replacing the single-site by a cluster of sites.
DMFT - General features

- Exact for $d \rightarrow \infty$
- For finite $d$, use the approximation $\Sigma(k, i\omega_n) \approx \Sigma(i\omega_n)$. 

Free Fermi gas is recovered when the interaction is switched off. At $U \rightarrow 0$ DMFT reproduces first order perturbation theory. Gives the correct result in the atomic limit, $U \rightarrow \infty$. The approximation $\Sigma(k, i\omega_n) \approx \Sigma(i\omega_n)$ can be relaxed replacing the single-site by a cluster of sites.
DMFT - General features

- Exact for $d \rightarrow \infty$
- For finite $d$, use the approximation $\Sigma(k, i\omega_n) \approx \Sigma(i\omega_n)$.
- Free Fermi gas is recovered when the interaction is switched off.
**DMFT - General features**

- Exact for $d \to \infty$
- For finite $d$, use the approximation $\Sigma(k, i\omega_n) \approx \Sigma(i\omega_n)$.
- Free Fermi gas is recovered when the interaction is switched off.
- At $U \to 0$ DMFT reproduces first order perturbation theory.
DMFT - General features

- Exact for $d \rightarrow \infty$
- For finite $d$, use the approximation $\Sigma(k, i\omega_n) \approx \Sigma(i\omega_n)$.
- Free Fermi gas is recovered when the interaction is switched off.
- At $U \rightarrow 0$ DMFT reproduces first order perturbation theory.
- Gives the correct result in the atomic limit, $U \rightarrow \infty$. 
**DMFT - General features**

- Exact for $d \to \infty$
- For finite $d$, use the approximation $\Sigma(k, i\omega_n) \approx \Sigma(i\omega_n)$.
- Free Fermi gas is recovered when the interaction is switched off.
- At $U \to 0$ DMFT reproduces first order perturbation theory.
- Gives the correct result in the atomic limit, $U \to \infty$.
- The approximation $\Sigma(k, i\omega_n) \approx \Sigma(i\omega_n)$ can be relaxed replacing the single-site by a cluster of sites.
Solving the impurity problem

The “free” impurity Green’s function $G_0$ is approximated by the function

$$G_0(i\omega_n)^{-1} = i\omega_n + \mu - \sum_p \frac{V_p^2}{i\omega_n - \tilde{\epsilon}_p}$$

which corresponds to the Anderson Hamiltonian

$$\mathcal{H}_{\text{And}} = \sum_{p \geq 2, \sigma} \tilde{\epsilon}_p a_p^{\dagger} a_{p\sigma} + \sum_{p \geq 2, \sigma} V_p (a_{p\sigma}^\dagger c_\sigma + c_\sigma^\dagger a_{p\sigma}) + Un^\uparrow n^\downarrow$$

For small number of auxiliary fields $a_{p\sigma}$ this Hamiltonian can be solved using standard diagonalization methods, or for $T = 0$ the Lanczos method.

M. Caffarel and W. Krauth, PRL 72, 1545 (1994)
Fermi Gas with a Contact interaction

In order to apply the DMFT to the Fermi Gas Hamiltonian

\[ H = -\frac{\hbar^2}{2m} \sum_\sigma \int dx \psi_\sigma^\dagger(x) \nabla^2 \psi_\sigma(x) + \frac{1}{2} V_0 \sum_\sigma \int dx \psi_\sigma^\dagger(x) \psi_{-\sigma}^\dagger(x) \psi_\sigma(x) \psi_{-\sigma}(x) \]

One has to become “griddy”, so

\[ x \rightarrow a n \; ; \; p \rightarrow \frac{2\pi}{Na} k \]

\[ \psi_\sigma(x) \rightarrow (a)^{3/2} \psi_{n\sigma} \]

and

\[ \{\psi_{n\sigma}, \psi_{n\sigma}^\dagger\} = \delta_{nn'} \delta_{\sigma\sigma'} \]
The Lattice Hamiltonian

The discretization leads to

\[ H = -\frac{\hbar^2}{2ma^2} \sum_{\sigma} \sum_{nn'} D_{nn'} \psi_{n\sigma}^{\dagger} \psi_{n'\sigma} + \frac{1}{2} \frac{V_0}{a^3} \sum_{\sigma n} \psi_{n\sigma}^{\dagger} \psi_{n-\sigma}^{\dagger} \psi_{n\sigma} \psi_{n-\sigma} \]

The spectra of the free Hamiltonian is given by

\[ \epsilon_p = \frac{\hbar^2}{ma^2} \Delta_p ; \quad \Delta_p = 2 \sum_i \sin^2 \frac{p_i}{2} \]

\( H \) contains the parameter \( V_0 \) that should be connected to the scattering length

Papenbrock & Bertsch, PRC 59, 2052 (1999)

\[ \frac{1}{4\pi a_s} = \frac{1}{V_0} + \frac{C}{2a} = \frac{1}{V_0} + \Lambda_K \frac{C}{4\pi} \]

where

\[ C = \int \frac{dp}{(2\pi)^3} \frac{1}{\Delta_p} \approx 0.5048 \]

and \( \Lambda_K = 2\pi/a \) is the momentum cutoff.
The Effective Range

The effective range is given by \( r_{eff} \approx \frac{4}{\pi \Lambda_K} = \frac{2a}{\pi^2} \).

In the unitary regime we would like

\[ r_{eff} k_F \ll 1 \]

or

\[ \frac{2a}{\pi^2} \sqrt{\frac{3\pi^2 \langle n \rangle}{a^3}} \approx \frac{2}{\pi} \sqrt{\langle n \rangle} \ll 1 \]

Here \( \langle n \rangle \) is the number of particles per site.
The Effective Range

The effective range is given by \( r_{eff} \approx \frac{4}{\pi \Lambda K} = \frac{2a}{\pi^2} \).
In the unitary regime we would like

\[ r_{eff} k_F \ll 1 \]

or

\[ \frac{2a}{\pi^2} \sqrt{\frac{3\pi^2 \langle n \rangle}{a^3}} \approx \frac{2}{\pi} \frac{3}{\langle n \rangle} \ll 1 \]

Here \( \langle n \rangle \) is the number of particles per site.

In practice

\[ 0.1 \geq \langle n \rangle \geq 0.01 \]

so

\[ 0.3 \geq r_{eff} k_F \geq 0.14 \]
Energy and density

The DMFT yields $\Sigma(i\omega_n)$, and

$$G(k, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma(i\omega_n)}$$

The density and energy can be calculated through the Matsubara sums,

$$\langle n \rangle = \frac{1}{\beta} \sum_{\sigma k} \sum_{i\omega_n = -\infty}^{\infty} e^{i0^+} G(k, i\omega_n)$$

$$\langle H \rangle = \frac{1}{2} \frac{1}{\beta} \sum_{\sigma k} \sum_{i\omega_n = -\infty}^{\infty} e^{i0^+} (i\omega_n + \epsilon_k + \mu) G(k, i\omega_n)$$

The density can be calculated directly from the impurity action. If $\mathcal{G} = G_{ii}$ this two results should coincide. However, the best we can hope for is $\mathcal{G} \approx G_{ii}$. 
**Evaluation of the Matsubara sums**

- Create a Pade approximation for $\Sigma$,

$$\Sigma^{Pade}(i\omega_n) = \frac{P(i\omega_n)}{Q(i\omega_n)} = \frac{\sum_{j=0}^{n} a_j (i\omega_n)^j}{\sum_{l=0}^{n} b_l (i\omega_n)^l}$$

- Use the Pade approximation and evaluate analytically the density, $\langle n \rangle_{Pade}$, and the energy $\langle H \rangle_{Pade}$.

- For a limited range of low frequencies calculate the difference

$$\delta\langle n \rangle = \frac{1}{\beta} \sum_{\sigma k} \sum_{i\omega_n = -i\omega_N} \left( \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma} - \frac{1}{i\omega_n + \mu - \epsilon_k - P/Q} \right)$$

- Finally,

$$\langle n \rangle = \langle n \rangle_{Pade} + \delta\langle n \rangle$$

$$\langle H \rangle = \langle H \rangle_{Pade} + \delta\langle H \rangle$$
The Pade Approximation

In the limit \( \omega \to \infty \), \( G \to 1/\omega \).
\[ \Rightarrow \] the order of the polynomials \( P, Q \) should be equal.

For the Pade approximation the Matsubara sums can be evaluated analytically

\[
\sum_{i\omega_n=-\infty}^{\infty} e^{i\omega_n^+} \frac{1}{i\omega_n + \mu - \epsilon - P/Q} = \sum_{p=1}^{n+1} \text{Res} \left( \frac{Q(\omega_p)}{R(\omega_p)} \right) \frac{\beta}{e^{\beta \omega_p} + 1}
\]

where

\[ R(\omega) = (\omega + \mu - \epsilon)Q(\omega) - P(\omega) \]

and \( \omega_p \) are the roots of \( R(\omega) \).
Numerical Results, $T = 0$

Notations

- Energy cutoff - $\Lambda_E$.
- Momentum cutoff - $\Lambda_K = \sqrt{2\Lambda_E}$.
- Grid size - $a = \frac{2\pi}{\Lambda_K}$.
- $n_s$ is the number of species in the Anderson model.
Free Fermi Gas

The ”impurity” and the “Lattice” densities in comparison to free Fermi gas.

\[ V_0=0, \mu=0.1, n_s=8 \]
The weak coupling regime

DMFT in comparison to perturbation theory.

\[ E/N = \epsilon_{FG} \left( 1 + \frac{10}{9\pi} k_F a_s + \frac{4(11 - 2\log 2)}{21\pi^2} (k_F a_s)^2 + \ldots \right) \]
The weak coupling regime

DMFT in comparison to perturbation theory.

\[ E/N = \epsilon_{FG} \left( 1 + \frac{10}{9\pi} k_F a_s + \frac{4(11 - 2\log2)}{21\pi^2} (k_F a_s)^2 + \ldots \right) \]

DMFT normalized to 1 at \( a_s = 0 \)
The strong coupling regime

Particle density at $a_s \rightarrow \infty$

There is no phase transition. Unlike static mean field theory.

The strong coupling regime

Particle density at $a_s \rightarrow \infty$

$\Rightarrow$ There is no phase transition. Unlike static mean field theory.

The strong coupling regime

Particle density at $\mu = 0.1$

DMFT, $n_s=8$

$\Lambda_E = 6$
$\Lambda_E = 8$
$\Lambda_E = 10$
The strong coupling regime

Particle density at $\mu = 0.1$

DMFT, $n_s=8$

$\Lambda_E = 6$
$\Lambda_E = 8$
$\Lambda_E = 10$

Density $\langle n \rangle / a^3$

$1/(a_s k_F)$
The strong coupling regime

Energy per particle at $\mu = 0.1$

![Graph showing the energy per particle as a function of $1/(a_s k_F)$ for different values of $\Lambda_E$. The graph illustrates the behavior of the Fermi gas in Dynamic Mean Field Theory (DMFT) for $n_s = 4$.](image-url)
The strong coupling regime

Energy per particle at $\mu = 0.1$
The strong coupling regime

Energy per particle at $\mu = 0.1$

The Fermi gas in Dynamic Mean Field Theory

Nir Barnea (HU, INT)
The strong coupling regime

Renormalization?

Normalized x-axis: $C \approx 0.5048$, $\delta C \approx -0.091$

$a_s = 4\pi V_0 + \Lambda K (C + \delta C)$

The strong coupling regime

Renormalization?

\[ \frac{1}{a_s} = \frac{4\pi}{V_0} + \Lambda_K (C + \delta C) \]

“Normalized” x-axis:

\[ C \approx 0.5048 \]
\[ \delta C \approx -0.09 \]
The strong coupling regime

Renormalization?

"Normalized" x-axis:
\[ C \approx 0.5048 \]
\[ \delta C \approx -0.09 \]

\[
\frac{1}{a_s} = \frac{4\pi}{V_0} + \Lambda_K (C + \delta C)
\]
The strong coupling regime

Renormalization?

\[ \frac{1}{a_s} = \frac{4\pi}{V_0} + \Lambda_K (C + \delta C) \]

“Normalized” x-axis:

\[ C \approx 0.5048 \]

\[ \delta C \approx -0.09 \]
The strong coupling regime

Renormalization?

“Normalized” x-axis:
\( C \approx 0.5048 \)
\( \delta C \approx -0.09 \)

Conclusions

DMFT describes very accurately the Fermi gas in the weak coupling regime. In the strong coupling regime DMFT captures the general behaviour. Unitarity is not realized, the results depend on the lattice filling, $\langle n \rangle$. Can DMFT provide a new framework for analyzing nuclear physics?
Conclusions

DMFT describes very accurately the Fermi gas in the weak coupling regime.
## Conclusions

1. DMFT describes very accurately the Fermi gas in the weak coupling regime.
2. In the strong coupling regime DMFT captures the general behaviour.

Unitarity is not realized, the results depend on the lattice filling, \( \langle n \rangle \).

Can DMFT provide a new framework for analyzing nuclear physics?
Conclusions

1. DMFT describes very accurately the Fermi gas in the weak coupling regime.
2. In the strong coupling regime DMFT captures the general behaviour.
3. Unitarity is not realized, the results depend on the lattice filling, \langle n \rangle.
**The Fermi Gas in DMFT**

### Conclusions

1. DMFT describes very accurately the Fermi gas in the weak coupling regime.
2. In the strong coupling regime DMFT captures the general behaviour.
3. Unitarity is not realized, the results depend on the lattice filling, $\langle n \rangle$.

### and a question

Can DMFT provide a new framework for analyzing nuclear physics?