The Fermi gas in Dynamic Mean Field Theory

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Introduction

Dynamic Mean Field Theory (DMFT)

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

Georges and Kotliar, PRB **45**, 6479 (1992)

A. Georges, G. Kotliar, W. Krauth, M. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)

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Having Nuclear Physics in Mind

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- 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

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

For a simple cubic lattice

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

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

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

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At this limit

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

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

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

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

$$G_{\sigma}(\boldsymbol{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}} - \boldsymbol{\Sigma}_{\sigma}(\boldsymbol{k}, i\omega_n)} \quad ; \quad \omega_n \equiv \frac{(2n+1)\pi}{\beta}$$

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At the limit $d \longrightarrow \infty$

Momentum space

$$\Sigma_{\sigma}(\boldsymbol{k}, i\omega_n) \longrightarrow \Sigma_{\sigma}(i\omega_n)$$

The Fourier transform of the Green's function takes a simple dependence on $\boldsymbol{k}$,

$$G_{\sigma}(\boldsymbol{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_{\sigma}(i\omega_n)}$$

Coordinate space

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

The site-diagonal Green's function

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

The single-site impurity model

Consider the effective action

$$\begin{aligned} S_{eff} &= -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^\dagger_{i,\sigma}(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_{i,\sigma}(\tau') \\ &\quad + U\int_0^\beta d\tau\, n_{i\uparrow}(\tau)n_{i\downarrow}(\tau) \end{aligned} \tag{1}$$

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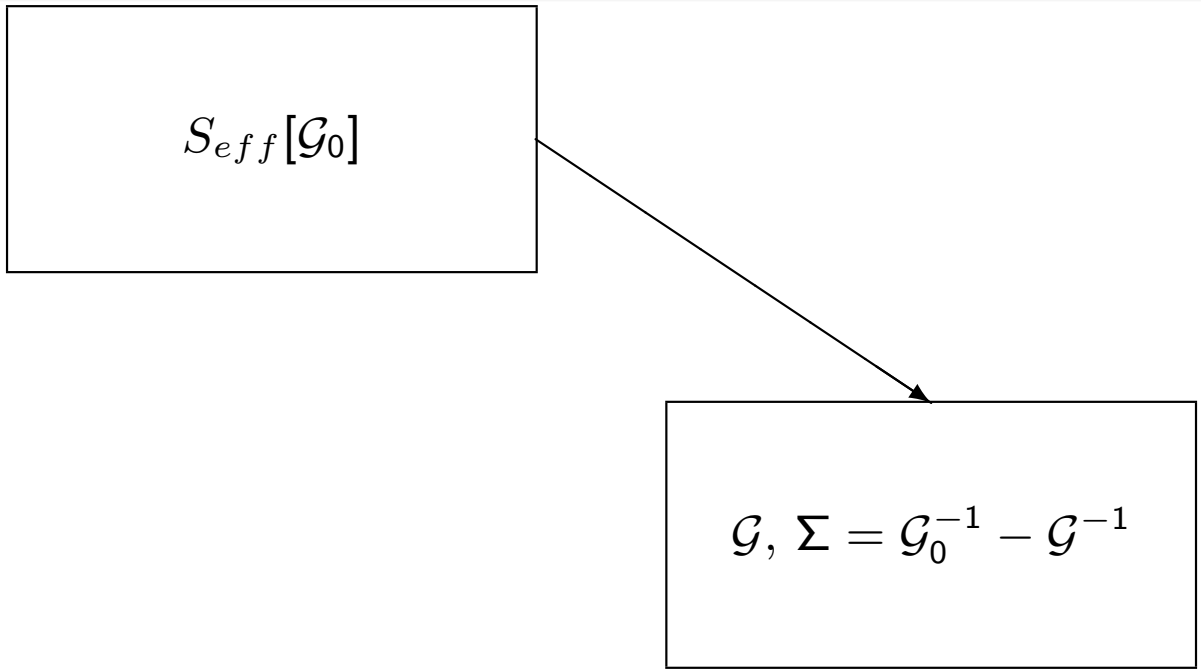
The connection to the physical lattice is made through the demand

$$\mathcal{G}(\tau-\tau') = G_{ii}(\tau-\tau')\,. \tag{4}$$

DMFT - The self-consistency condition

$$S_{eff}[\mathcal{G}_0]$$

DMFT - The self-consistency condition



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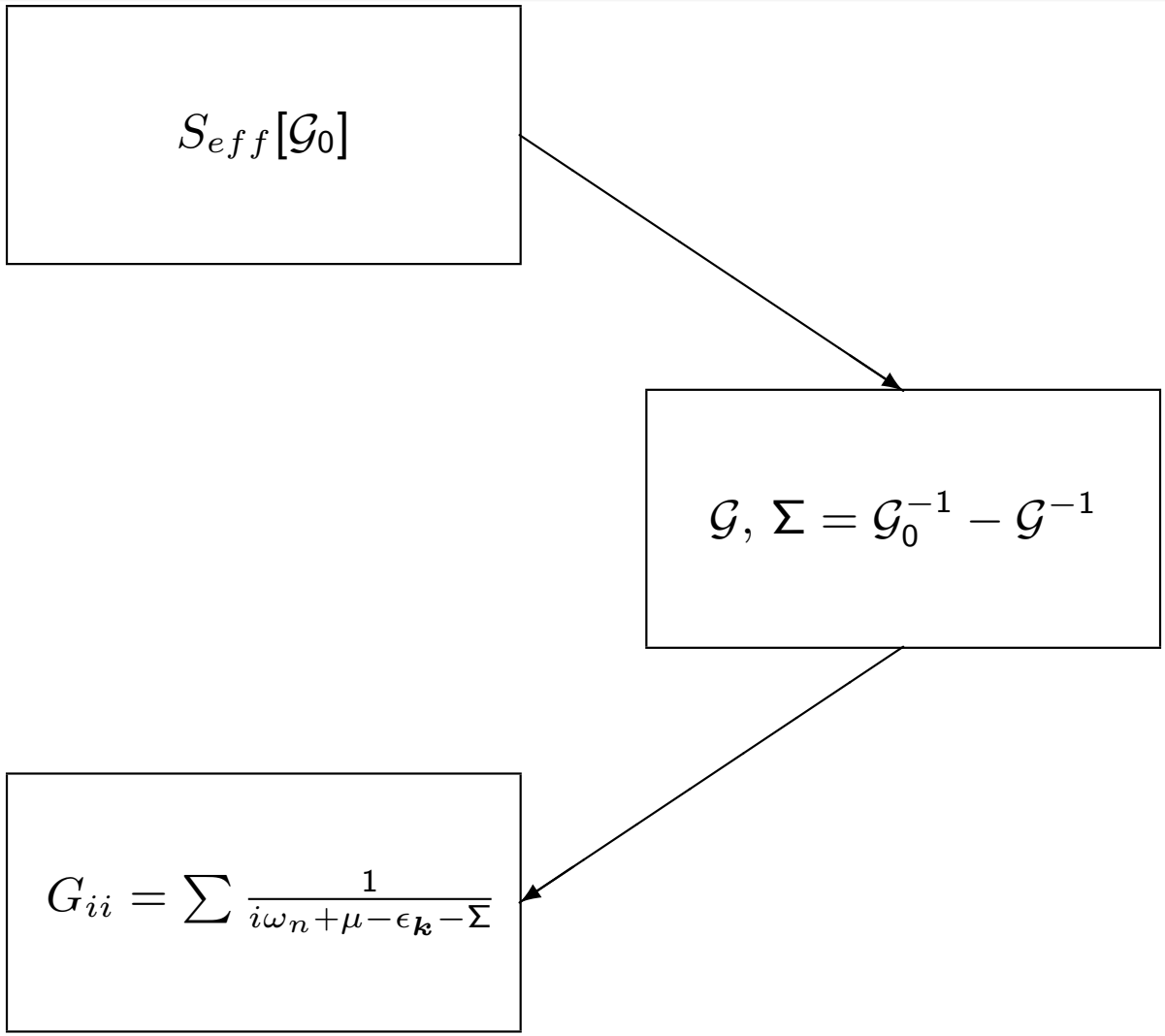

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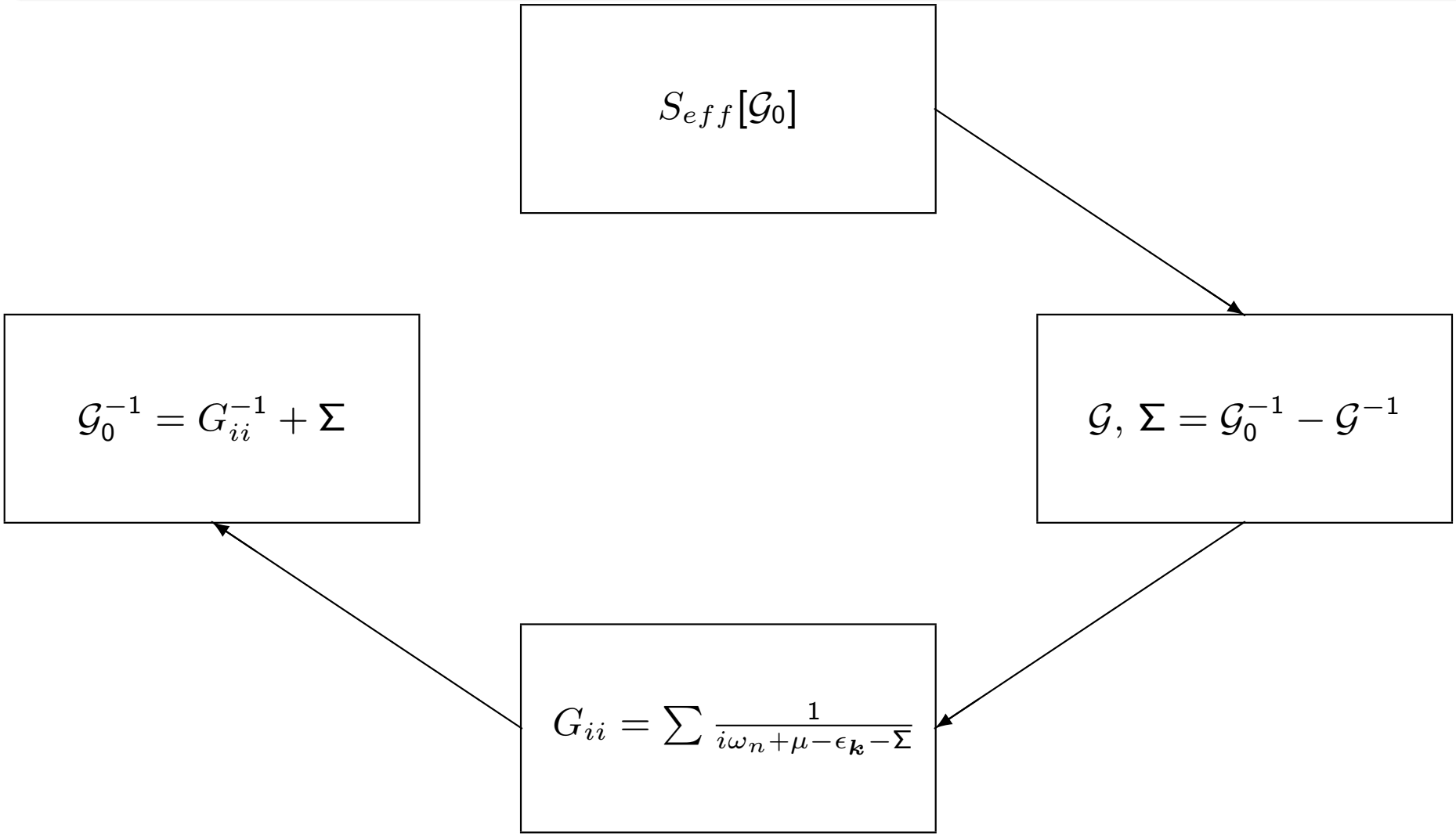

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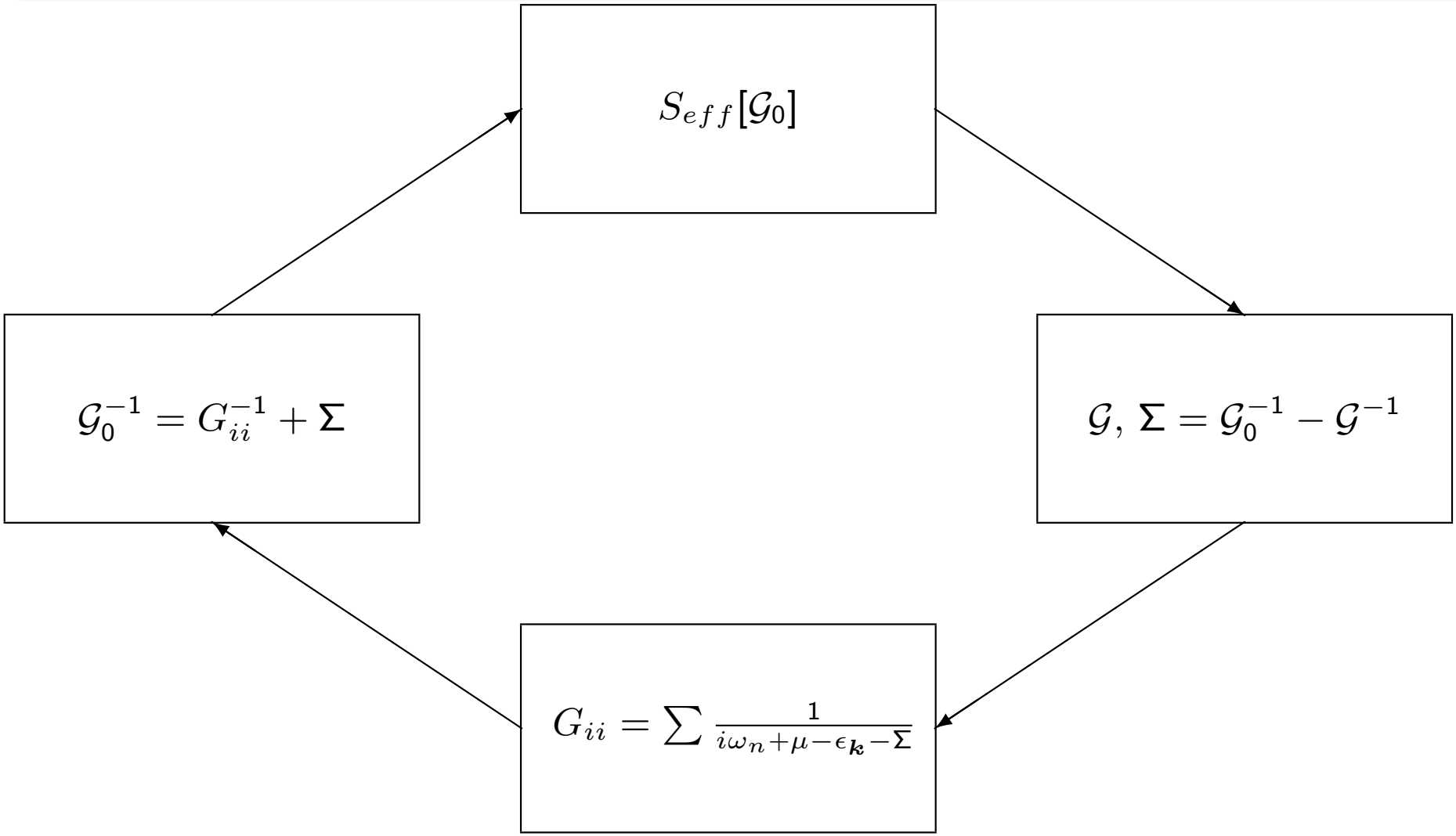

DMFT - General features

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- At $U \longrightarrow 0$ DMFT reproduces first order perturbation theory.
- Gives the correct result in the atomic limit, $U \longrightarrow \infty$.
- The approximation $\mathbf{\Sigma}(\boldsymbol{k}, i\omega_n) \approx \mathbf{\Sigma}(i\omega_n)$ can be relaxed replacing the single-site by a cluster of sites.

Solving the impurity problem

The "free" impurity Green's function $\mathcal{G}_0$ is approximated by the function

$$\mathcal{G}_0(i\omega_n)^{-1} = i\omega_n + \mu - \sum_p \frac{V_p^2}{i\omega_n - \tilde{\epsilon}_p}$$

which corresponds to the Anderson Hamiltonian

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

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

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\sum_\sigma \int d\boldsymbol{x}\psi^\dagger_\sigma(\boldsymbol{x})\nabla^2\psi_\sigma(\boldsymbol{x}) \\ &\quad + \frac{1}{2}V_0\sum_\sigma \int d\boldsymbol{x}\psi^\dagger_\sigma(\boldsymbol{x})\psi^\dagger_{-\sigma}(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})\psi_{-\sigma}(\boldsymbol{x}) \end{aligned}$$

One has to become "griddy", so

$$\boldsymbol{x} \longrightarrow a\boldsymbol{n} \quad ; \quad \boldsymbol{p} \longrightarrow \frac{2\pi}{Na}\boldsymbol{k}$$

$$\psi_\sigma(\boldsymbol{x}) \longrightarrow (a)^{3/2}\psi_{\boldsymbol{n}\sigma}$$

and

$$\{\psi_{\boldsymbol{n}\sigma}, \psi^\dagger_{\boldsymbol{n}\sigma}\} = \delta_{nn'}\delta_{\sigma\sigma'}$$

The Lattice Hamiltonian

The discretization leads to

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

The spectra of the free Hamiltonian is given by

$$\epsilon_{\boldsymbol{p}} = \frac{\hbar^2}{ma^2}\Delta_{\boldsymbol{p}} \quad ; \quad \Delta_{\boldsymbol{p}} = 2\sum_i \sin^2\frac{p_i}{2}$$

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

$$C = \int \frac{d\boldsymbol{p}}{(2\pi)^3}\frac{1}{\Delta_{\boldsymbol{p}}} \approx 0.5048$$

and $\Lambda_K = 2\pi/a$ is the momentum cutoff.

The Effective Range

The effective range is given by $r_{eff} \approx 4/\pi\Lambda_K = 2a/\pi^2$.
In the unitary regime we would like

$$r_{eff} k_F \ll 1$$

or

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

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

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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

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

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

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

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

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

1. Create a Pade approximation for Σ,

$$\Sigma^{Pade}(i\omega_n) = \frac{P(i\omega_n)}{Q(i\omega_n)} = \frac{\sum_0^n a_j (i\omega_n)^j}{\sum_0^n b_l (i\omega_n)^l}$$

2. Use the Pade approximation and evaluate analytically the density, $\langle n \rangle_{Pade}$, and the energy $\langle H \rangle_{Pade}$.
3. For a limited range of low frequencies calculate the difference

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

4. 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 $\omega \longrightarrow \infty$, $G \longrightarrow 1/\omega$.
$\Rightarrow$ the order of the polynomials P, Q should be equal.

For the Pade approximation the Matsubara sums can be evaluated analytically

$$\sum_{i\omega_n=-\infty}^{\infty} e^{i0^+} \frac{1}{i\omega_n + \mu - \epsilon - P/Q} = \sum_{p=1}^{n+1} Res\left(\frac{Q(\omega_p)}{R(\omega_p)}\right) \frac{\beta}{e^{\beta\omega_p}+1}$$

where

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

and ω_p are the roots of $R(\omega)$.

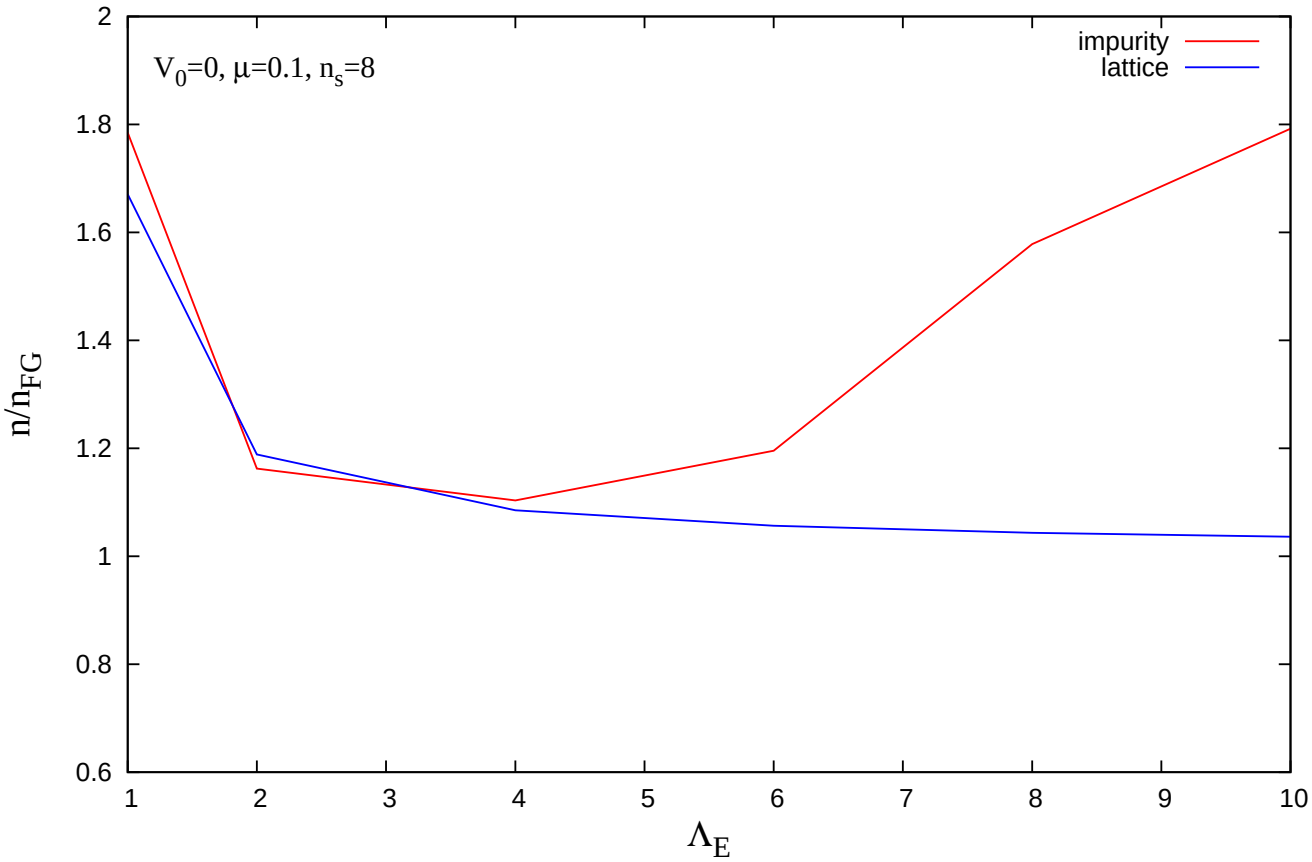
Numerical Results, $T = 0$

Notations

- Energy cutoff - Λ_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

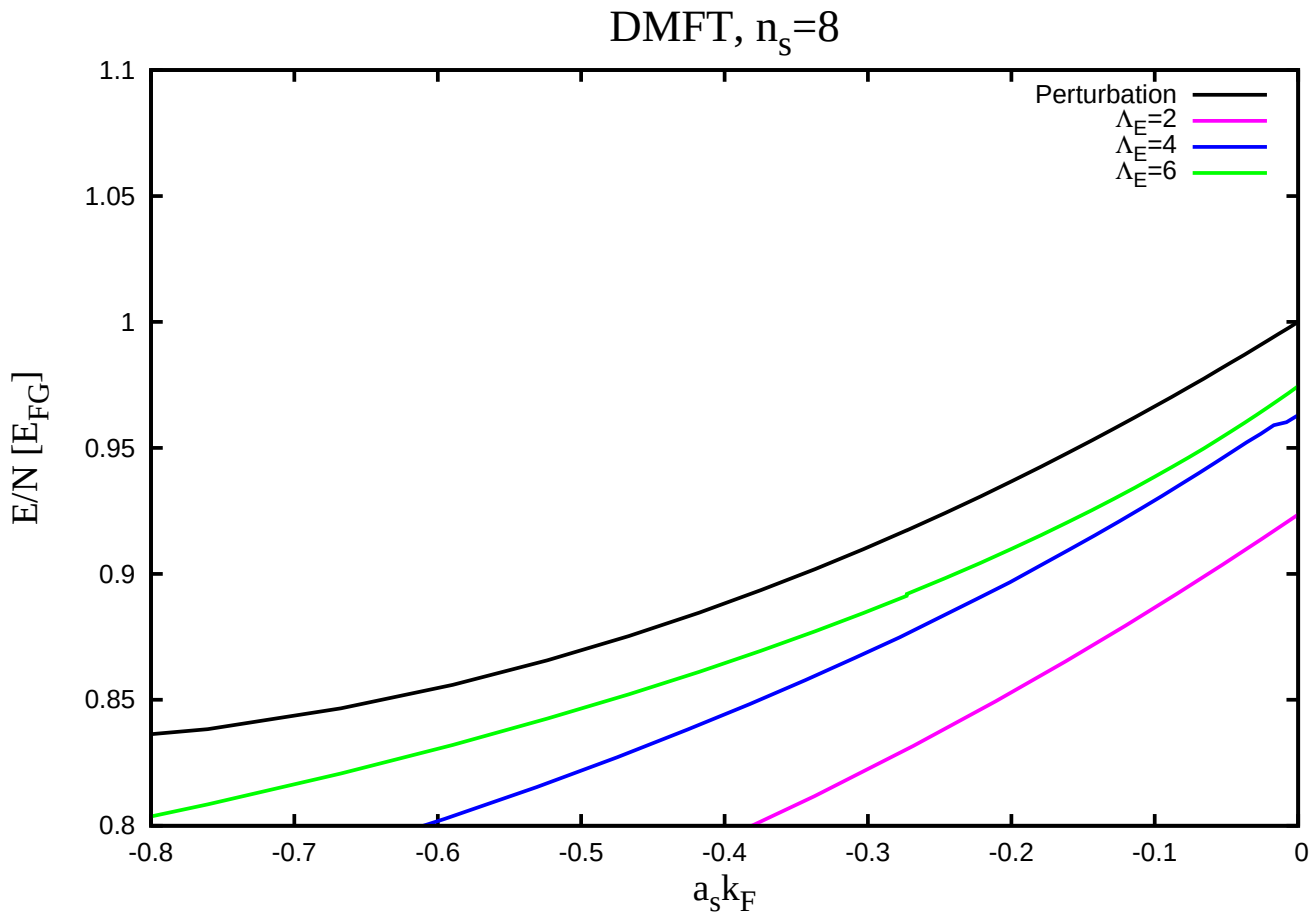
The "impurity" and the "Lattice" densities in comparison to free Fermi gas.



The weak coupling regime

DMFT in comparison to perturbation theory.

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



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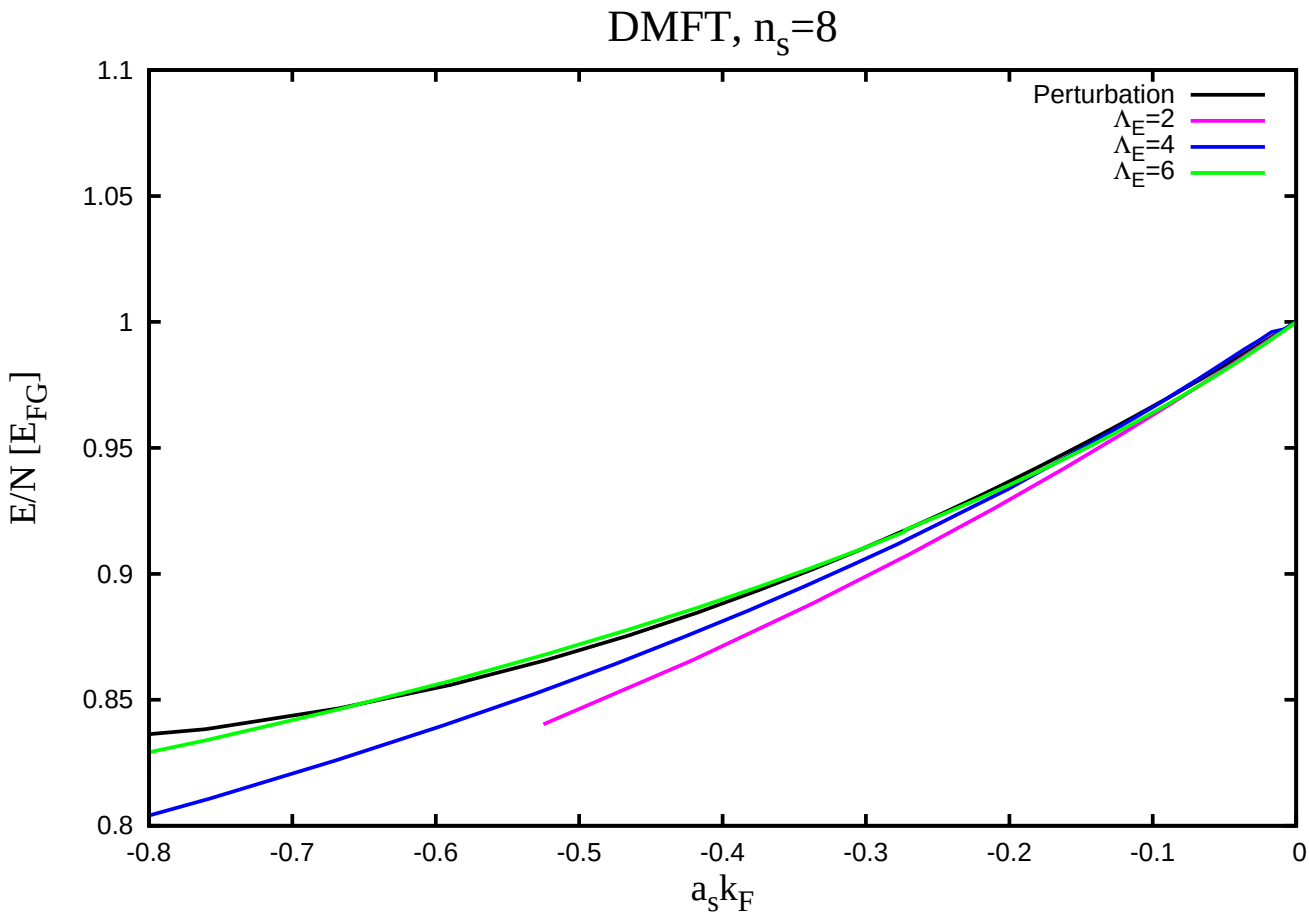
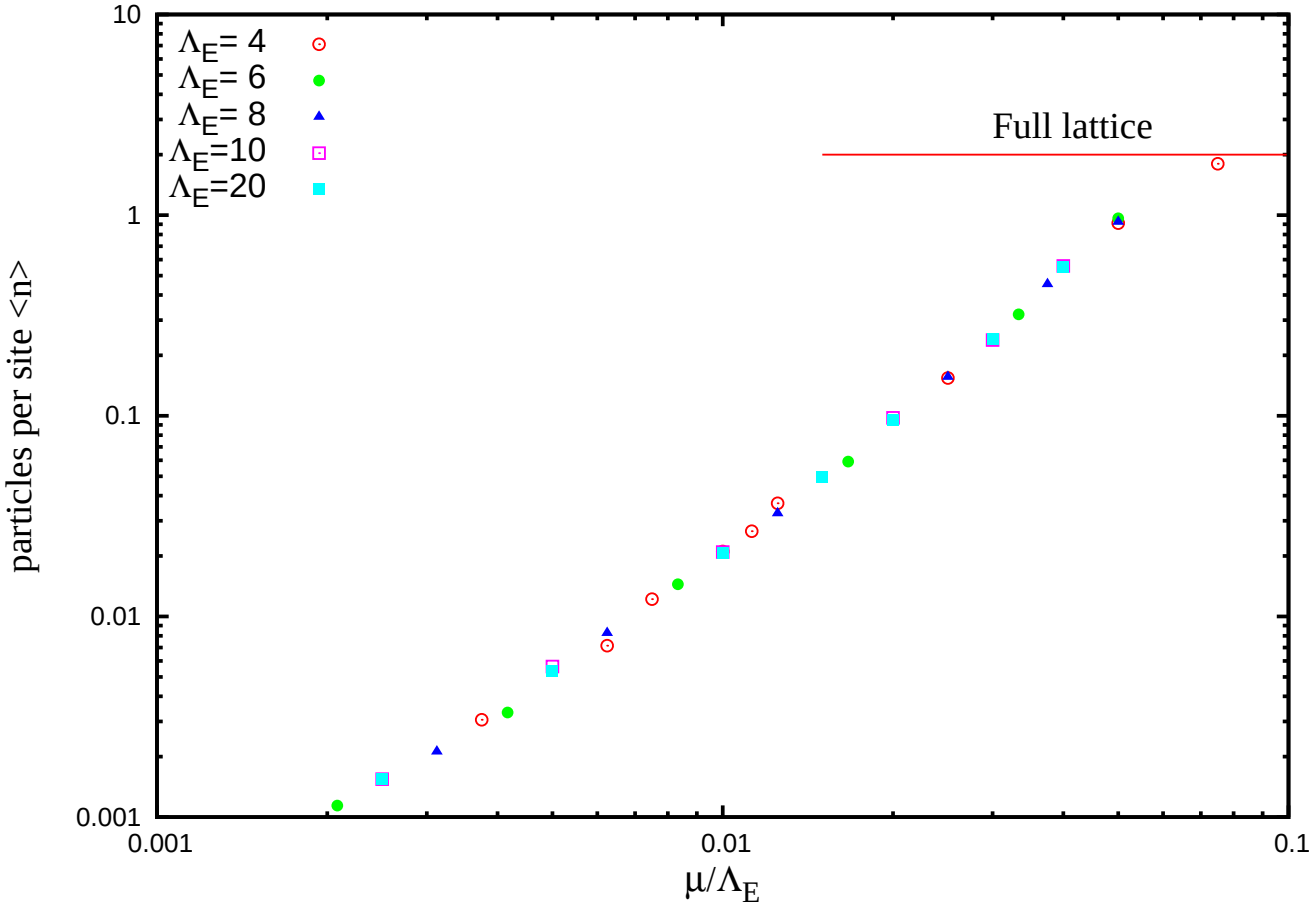


DMFT normalized to 1 at $a_s = 0$

Particle density at $a_s \longrightarrow \infty$



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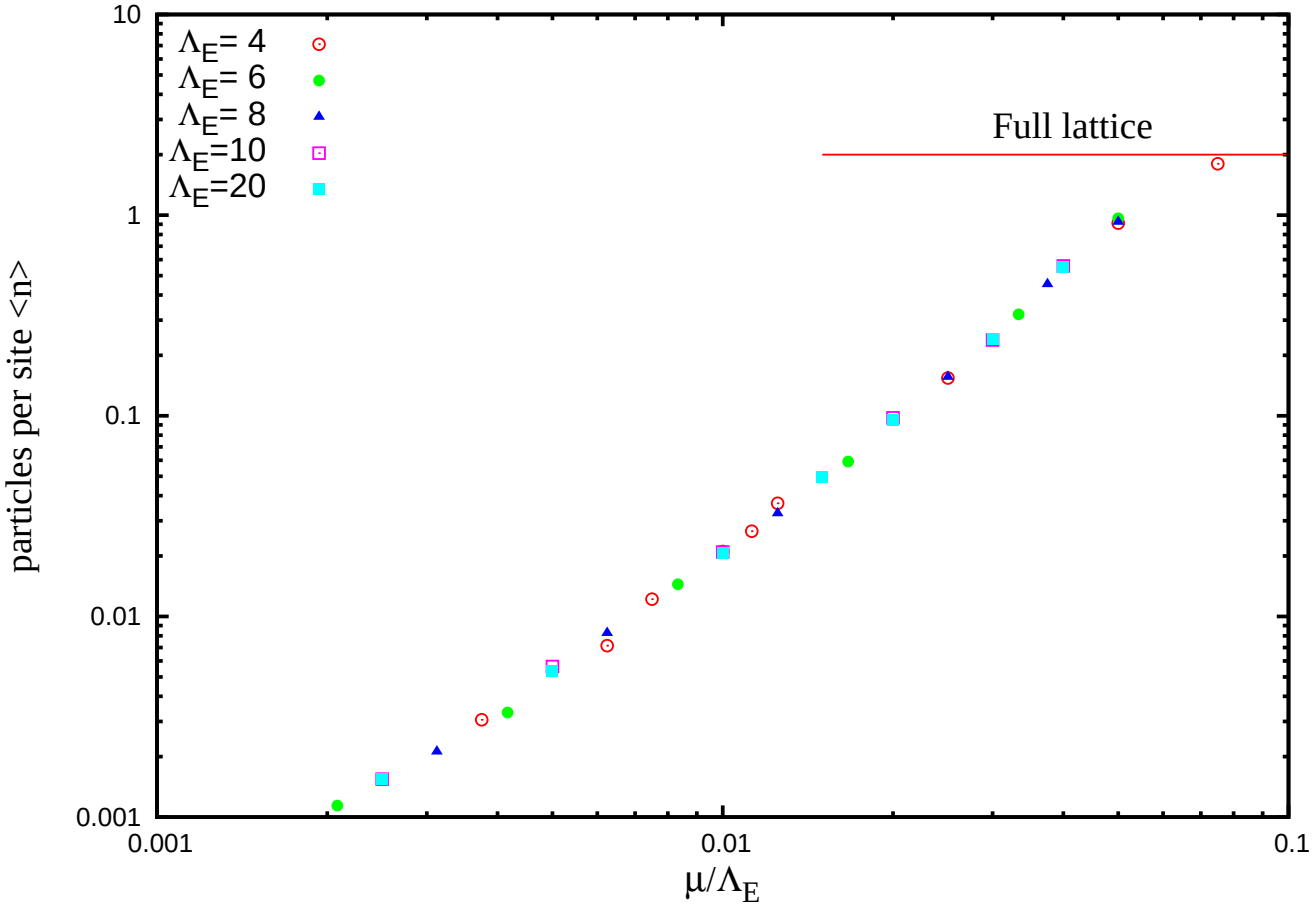
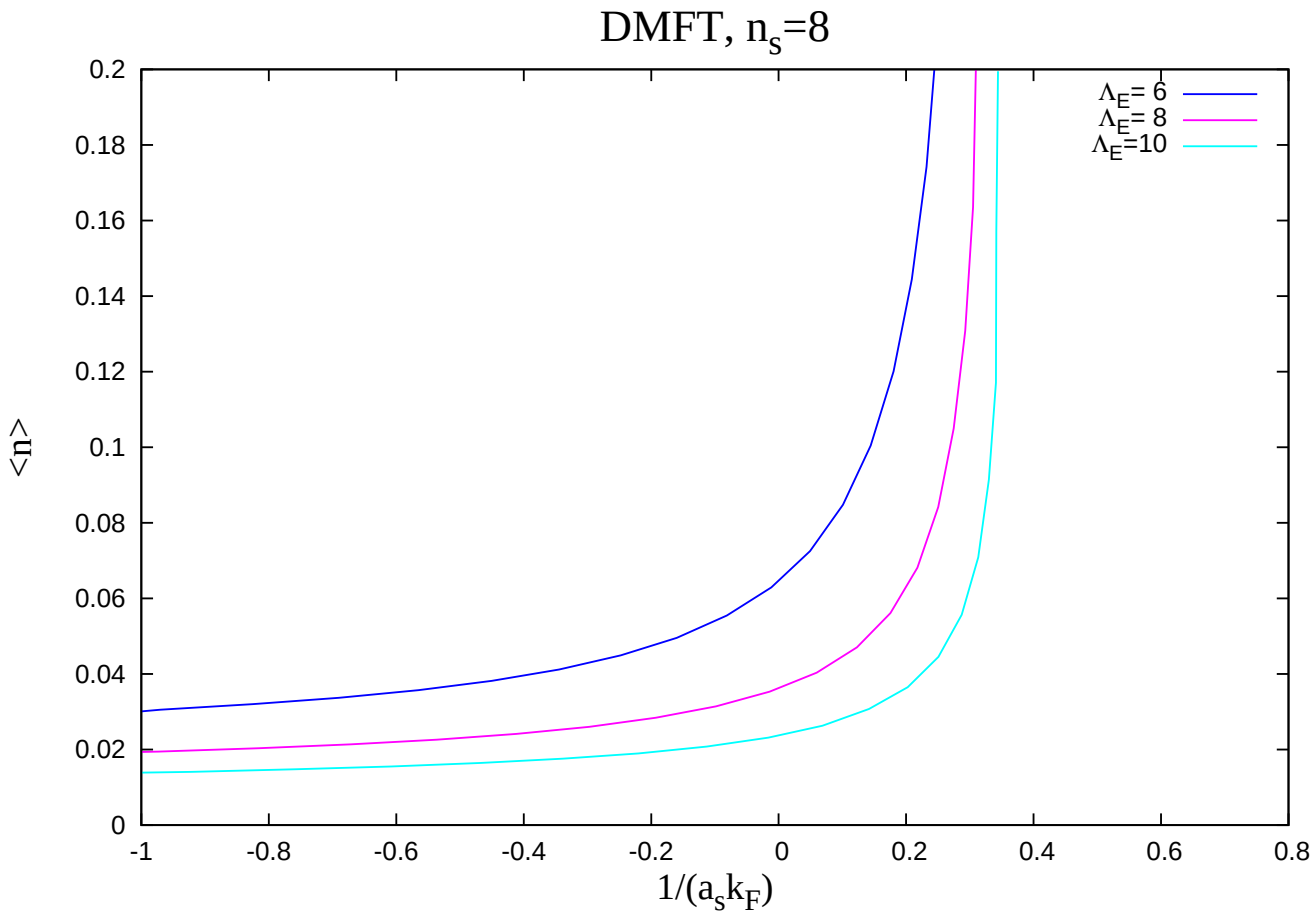


$\Rightarrow$ There is no phase transition. Unlike static mean field theory.

J. Chen and D. B. Kaplan, PRL **92**, 257002 (2004).

Particle density at $\mu = 0.1$



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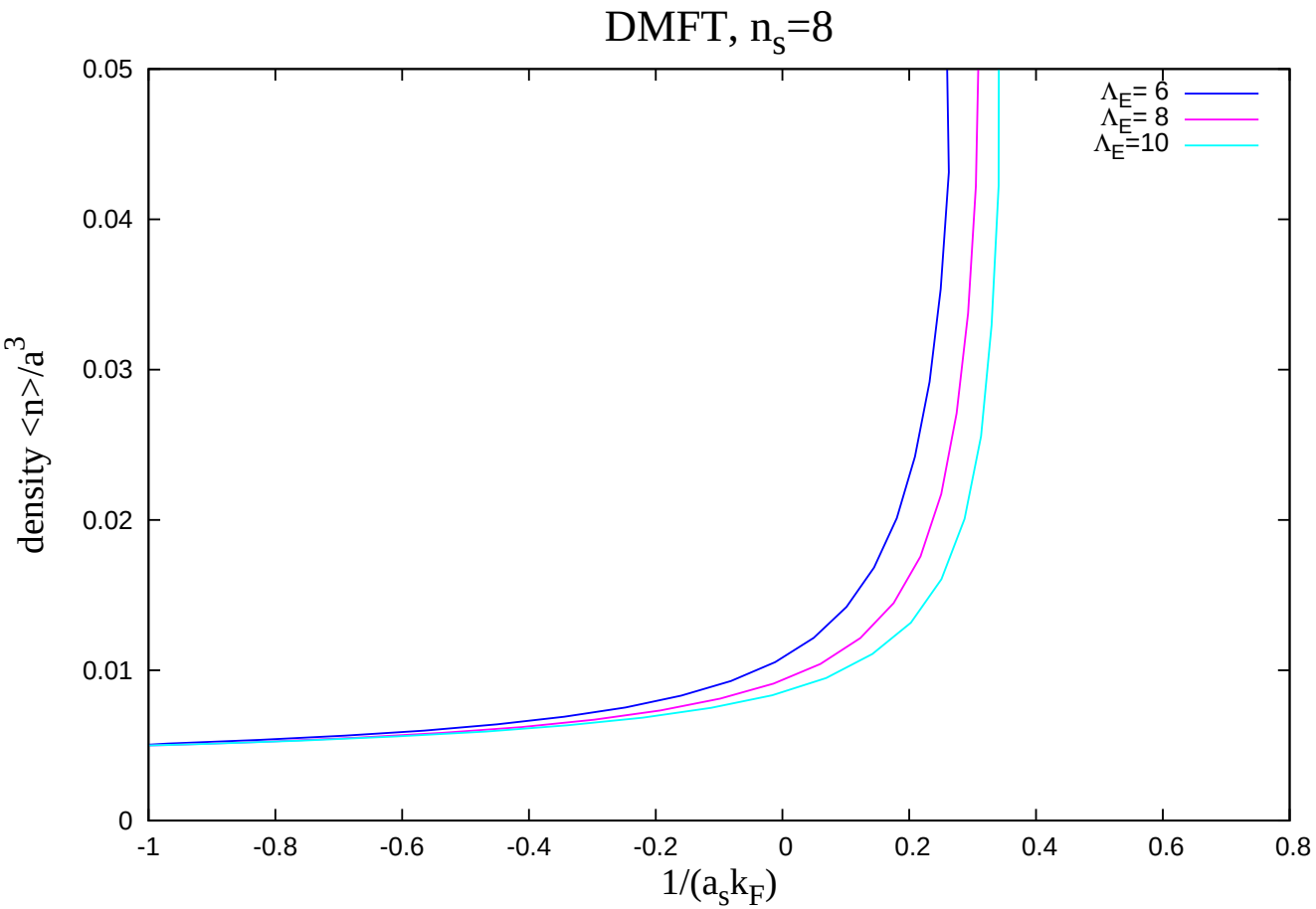

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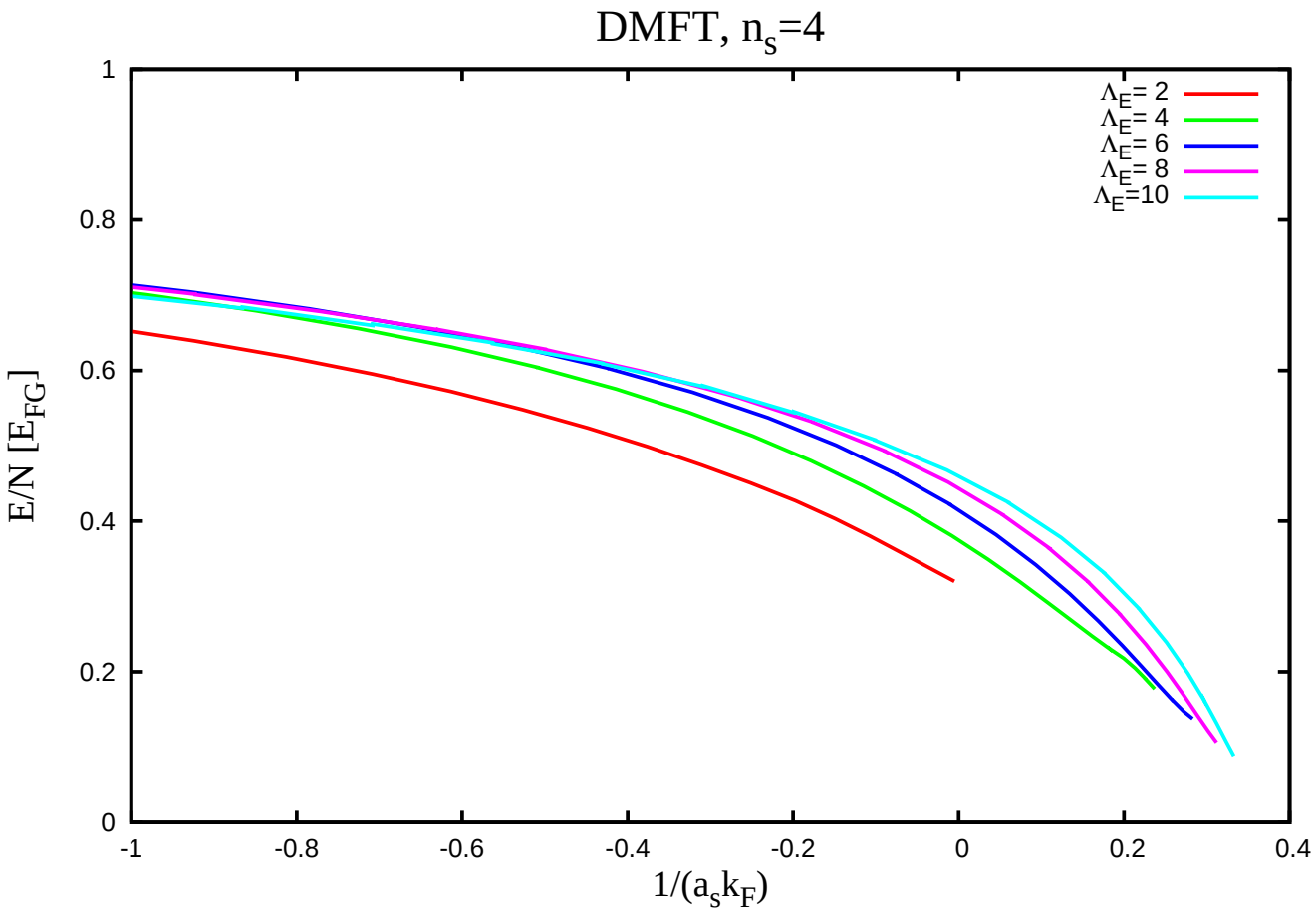

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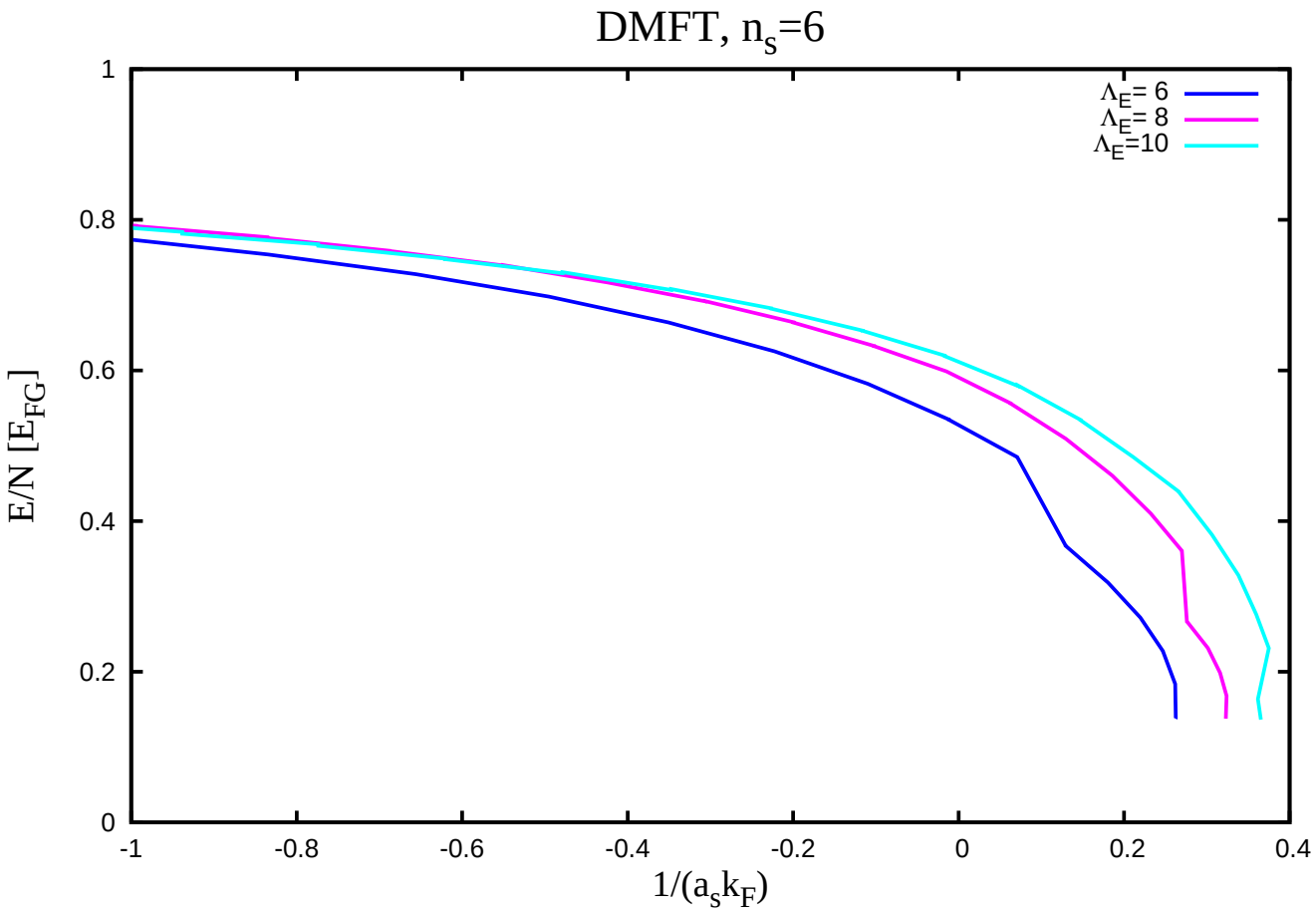

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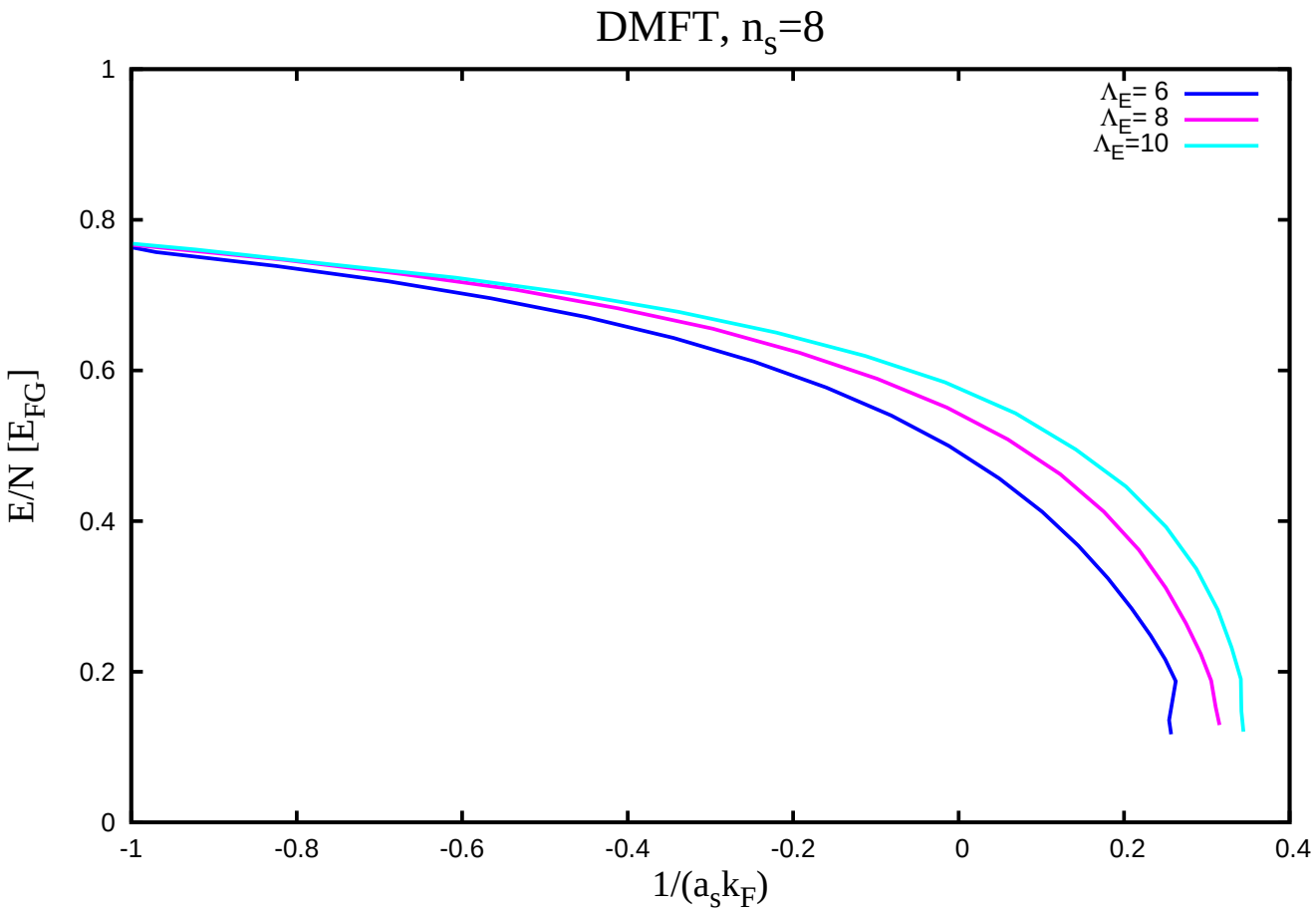
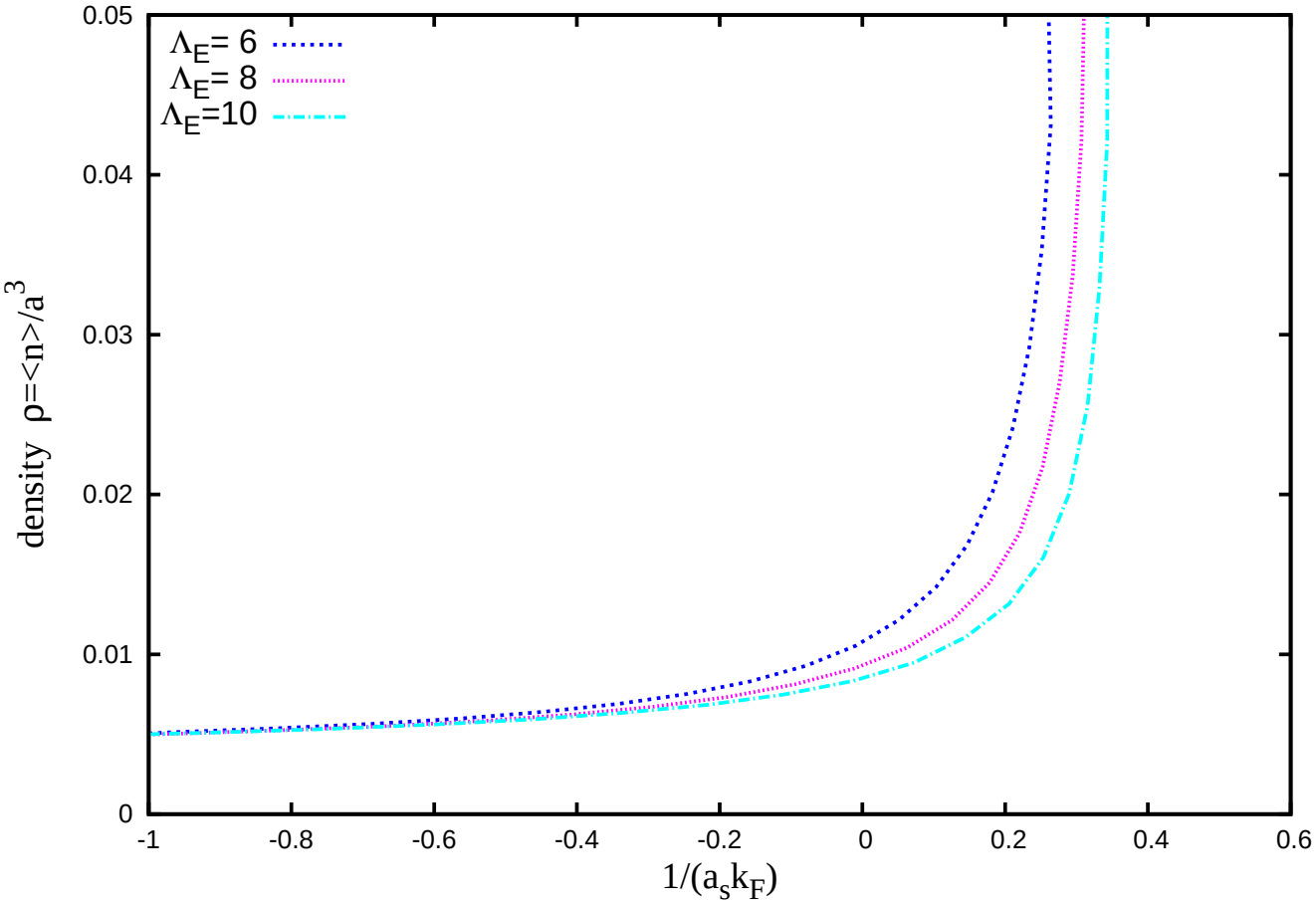


Renormalization?



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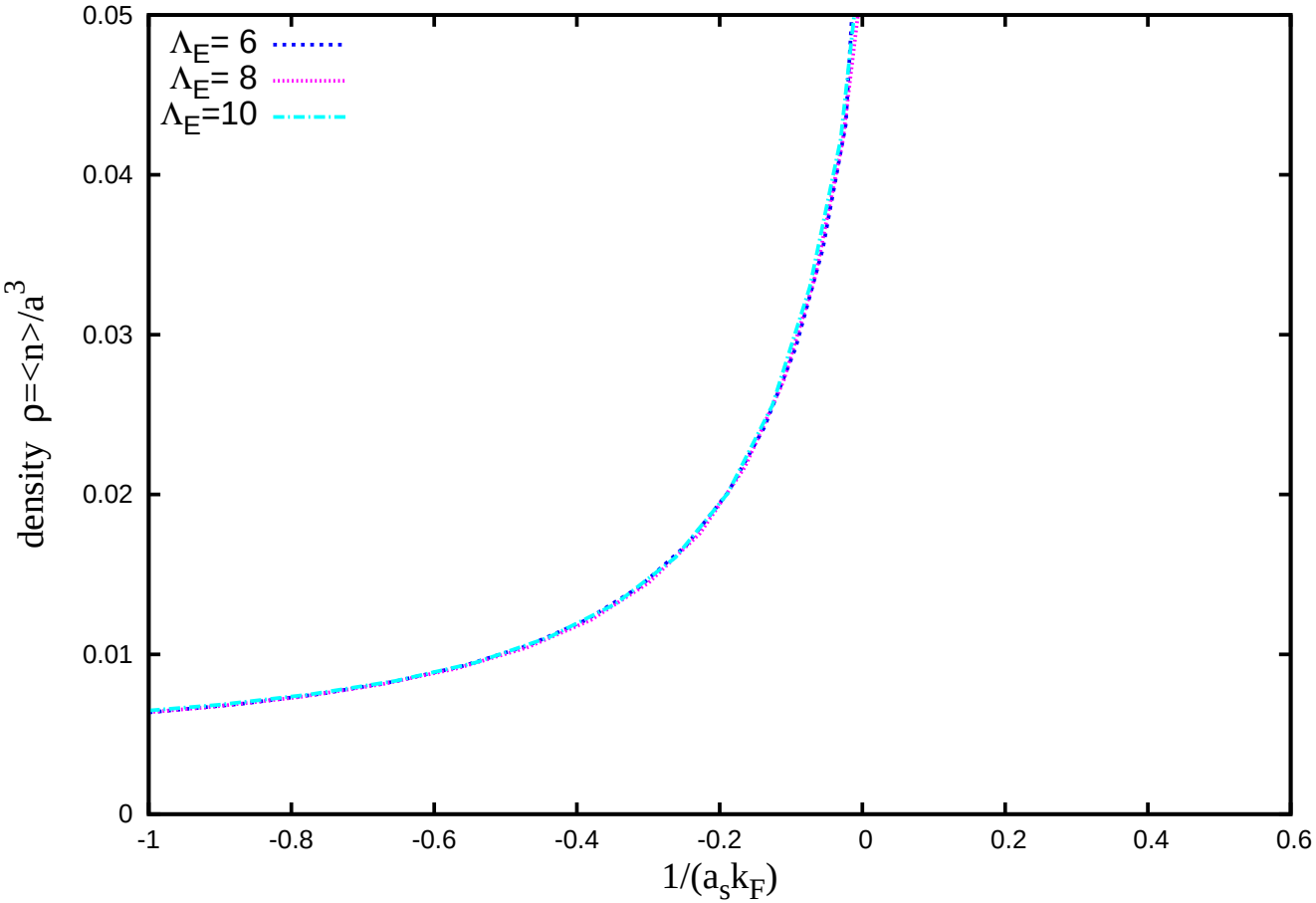

"Normalized" x-axis:
$C \approx 0.5048$
$\delta C \approx -0.09$

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

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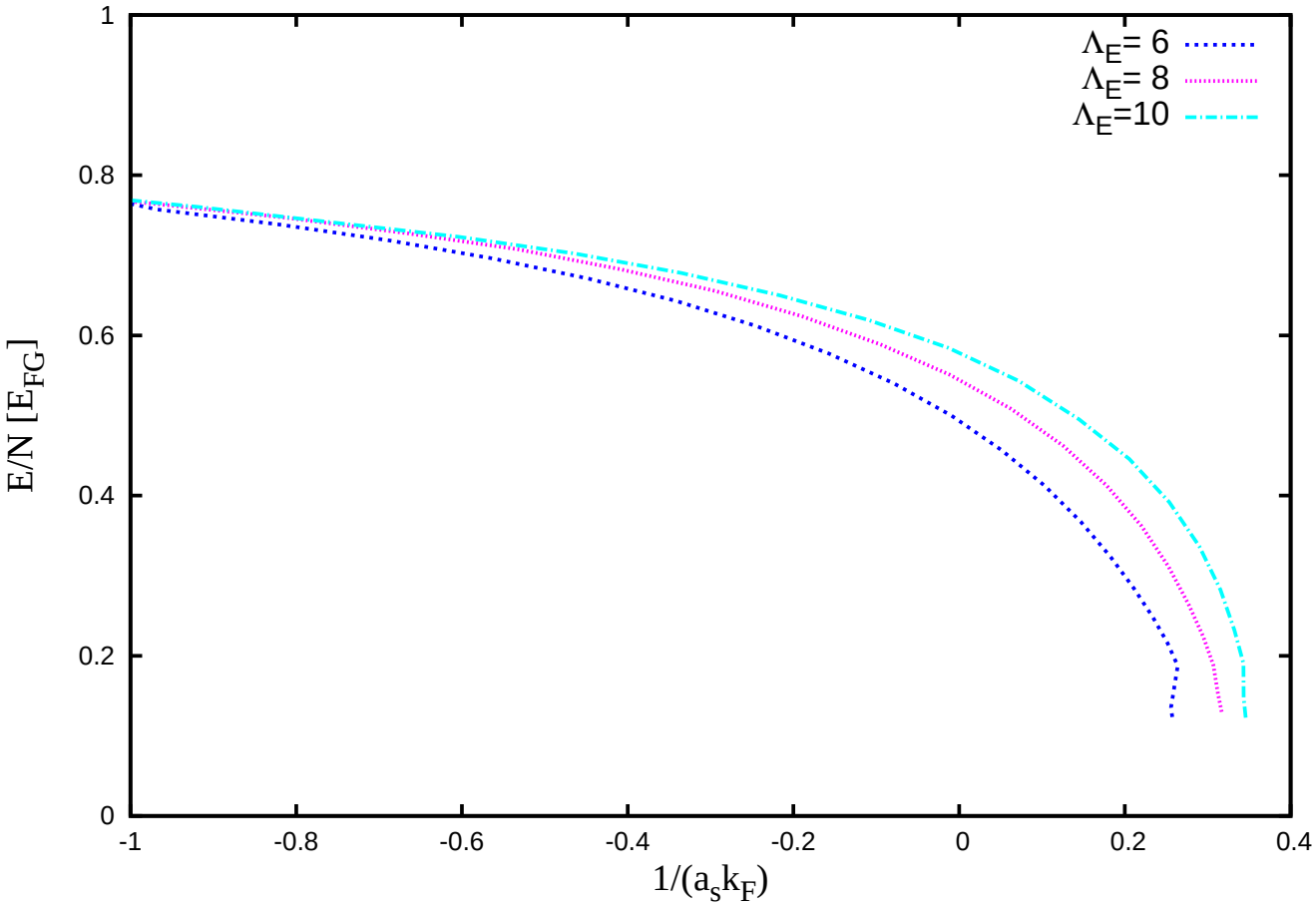

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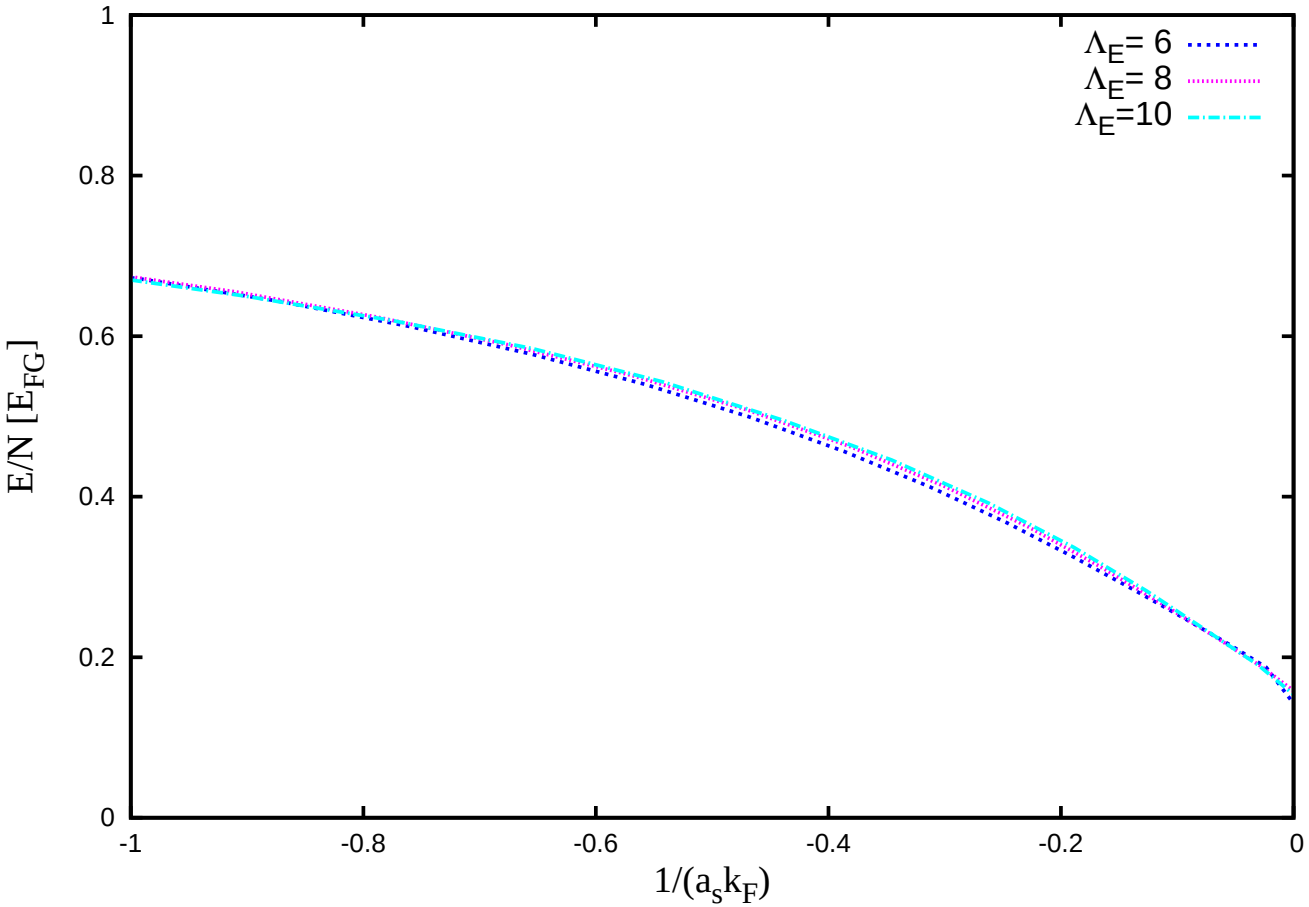

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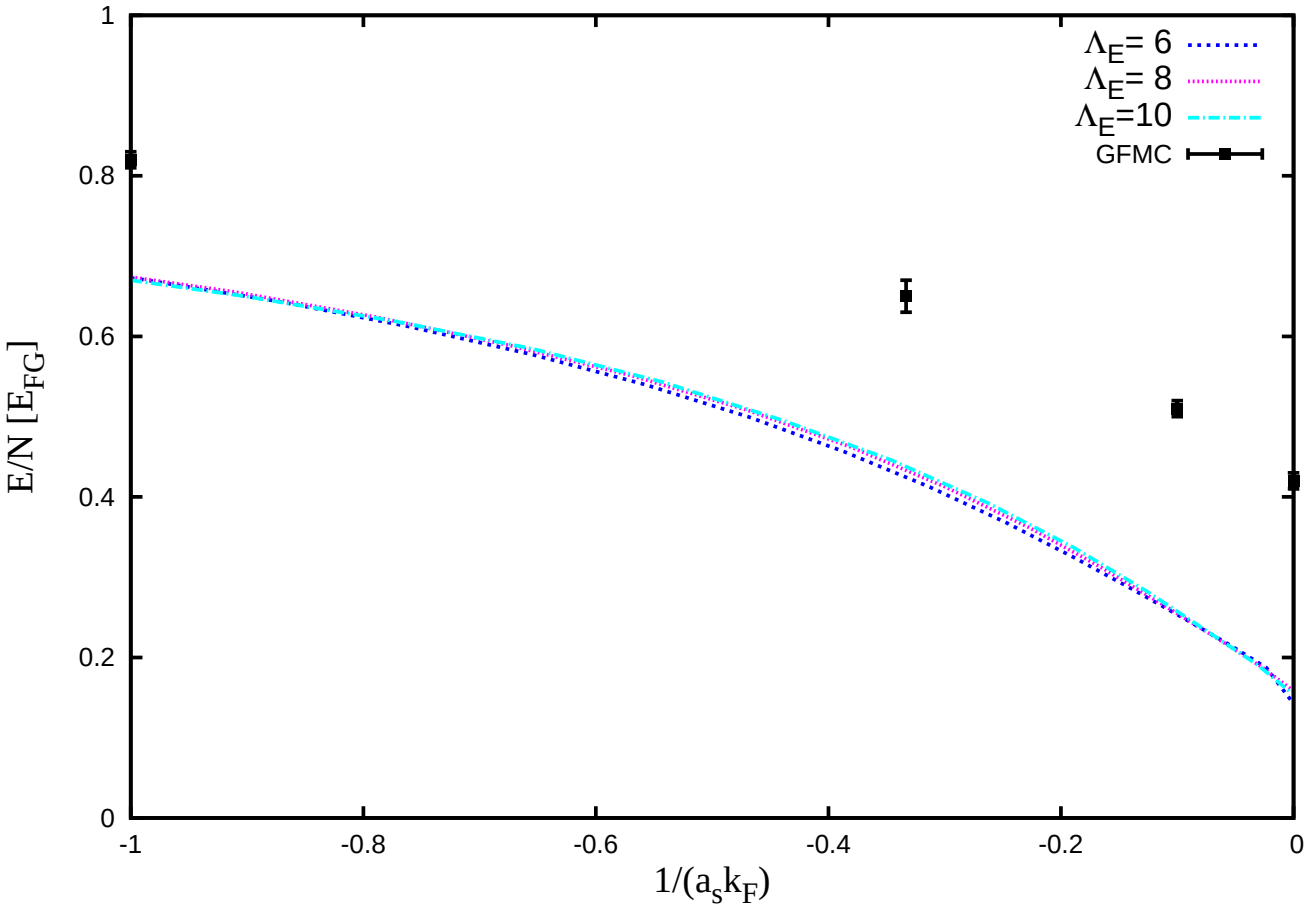

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GFMC - S. Y. Chang, V. R. Pandharipande, J. Carlson, and S. E. Schmidt, PRA. **70**, 043602 (2004).

Conclusions

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and a question

Can DMFT provide a new framework for analyzing nuclear physics?