Analytic calculation of an effective lattice theory

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July 06th 2015

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Our Group

- Me: Started August 2013

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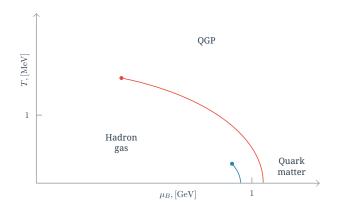
Introduction

The QCD Phase Diagram
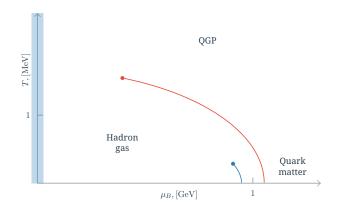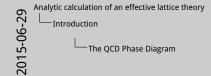

- Different approaches can access different regions
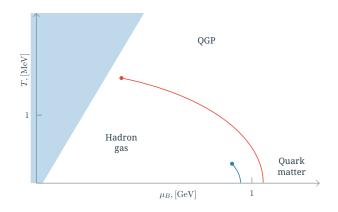
The QCD Phase Diagram

- Naïve reach of Lattice QCD

Lattice QCD cannot natively deal with a finite baryon chemical potential because that turns the quark determinant into a complex quantity. On top of that we get important exponential cancellations coming from the "sign problem", which will be addressed later in this talk.
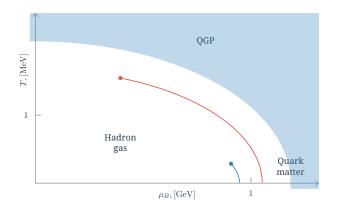
The QCD Phase Diagram

- Lattice QCD with additional methods (analytic continuation, reweighting,...)

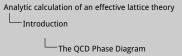There are various techniques available to study finite density systems. With reweighting one uses the $\mu = 0$ system to evolve the Monte Carlo, then uses the actual $\mu \neq 0$ to measure observables. One can also measure the system at imaginary chemical potential and then use analytic continuation to extrapolate the results for $\mu^2 < 0$ to $\mu^2 > 0$.

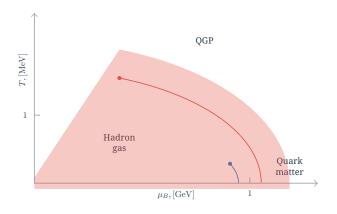# The QCD Phase Diagram

- Perturbation theory of QCD
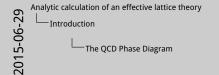
Perturbation theory can of course only handle QCD at extreme temperatures and chemical potential, regions where the thermodynamic energy is large enough to have the QCD coupling run to values small enough for perturbation theory to be valid.

The QCD Phase Diagram

- Region currently not accessible from first principles with traditional methods

The QCD Phase Diagram

- Region currently not accessible from first principles with traditional methods

Most of the interesting phase structure is still in areas inaccessible to first principles theoretical approaches.

Lattice QCD: Basics 1

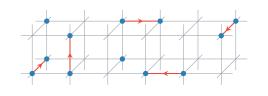Discretise space and time

Quarks

$$\mathcal{L}_F = \bar{\psi}(x)\left(i\gamma_\mu\partial^\mu + \gamma_\mu A^\mu\right)\psi(x) + m_q\bar{\psi}(x)\psi(x)$$

$$\downarrow\; x \to an$$

$$L_F \sim \sum_\mu \bar{\psi}(n)U_\mu(n)\psi(n+\mu) + m_q\bar{\psi}(n)\psi(n)$$
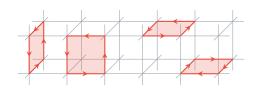
See that the $\psi(n)$ variables have a set position n, and are thus are associated with the different points on our lattice. The variables $U_\mu(n)$ have both a position n, and a direction μ. It can therefore for example be associated with to points, or more conveniently with the link between the two points.

This is what we mean when we say that in Lattice QCD the quarks live on the sites and the gluons on the links.

The first term in the QCD Lagrangian thus is a sort of directional nearest neighbour interaction, where the

interaction link itself is a variable.

Lattice QCD: Basics 2

Discretise space and time

Gluons

$$\mathcal{L}_G = \frac{1}{4} \operatorname{tr} F_{\mu\nu}(x) F^{\mu\nu}(x)$$

$$\downarrow x \to an$$

$$L_G \sim \beta \sum_{\mu,\nu} \operatorname{tr} U_\mu(n) U_\nu(n+\mu) U_\mu^\dagger(n+\nu) U_\nu^\dagger(n)$$

Lattice QCD: Basics 2

Discretise space and time

┌─ Gluons ──────────────────────

$$\mathcal{L}_G = \frac{1}{4} \text{tr} \, F_{\mu\nu}(x) F^{\mu\nu}(x)$$

$$\Big| \, x \to an$$

$$\mathcal{L}_G \sim \beta \sum_{\mu,\nu} \text{tr} \, U_\mu(n) U_\nu(n + \mu) U_\mu^\dagger(n + \nu) U_\nu^\dagger(n)$$

The link plaquette constites the smallest gauge invariant geometric quantity one can construct on the lattice using the group elements U. It is very similar to how one construct $F_{\mu\nu}$ in continuous Yang-Mills theory if one doesn't go the covariant derivative route.

Lattice QCD: Basics 3

Partition function

$$\mathcal{Z} = \int DU_\mu D\bar{\psi} D\psi \, \exp\left\{ -\bar{\psi} Q_{\text{uark}} \psi - S_{\text{gluon}} \right\}$$

$$= \int DU_\mu \det Q_{\text{uark}} \exp\left\{ -S_{\text{gluon}} \right\}$$

Measure observables by running a Monte Carlo simulation using

Monte Carlo weight

$$\det Q_{\text{uark}} \exp\left\{ -S_{\text{gluon}} \right\}$$

Lattice QCD: Basics 3

┌─ Partition function ──────────────
  $\mathcal{Z} - \int DU_\nu D\bar{\psi} D\psi \, \exp\left\{ -\bar{\psi} Q_{\text{quark}} \psi - S_{\text{gluon}} \right\}$

  $- \int DU_\nu \, \det Q_{\text{quark}} \, \exp\left\{ -S_{\text{gluon}} \right\}$

Measure observables by running a Monte Carlo
simulation using

┌─ Monte Carlo weight ──────────────
  $\det Q_{\text{quark}} \, \exp\left\{ -S_{\text{gluon}} \right\}$

When doing lattice simulations, the integral over the fermion fields are done analytically which results in the determinant of the quark matrix Q_{quark}. There are other ways of approaching this, but from a technical standpoint it is also convenient to get rid of the Grassmann-variables, as they are hard to deal with numerically. The remaining integral over the fields U_μ is a strongly coupled, highly dimensional integral that is almost impossible to solve in practice. Therefore we rather use the measure in the integral as a Monte Carlo weight, and can use a Monte Carlo simulation algorithm to evolve the system in a way that minimises the action, measuring observables along the way.

One does thus not calculate $\mathcal{Z}$ in Lattice QCD, but one calculates observables: $\langle O \rangle = \dfrac{1}{\mathcal{Z}} \int DU \, O(U) e^{-S}$

Lattice QCD: Challenges
Simulation cost

Counting the degrees of freedom of the system gives a staggering number

$$N = N_t \times N_x \times N_y \times N_z \times N_\gamma \times N_f \times N_c$$

Every simulation point must evaluate det Q_{uark}, which is a (sparse) $N \times N$ matrix

Lattice QCD: Challenges
Simulation cost

Counting the degrees of freedom of the system gives a staggering number

$$N = N_l \times N_s \times N_f \times N_c \times N_s \times N_f \times N_s$$

Every simulation point must evaluate $\det Q_{carlo}$, which is a (sparse) $N \times N$ matrix

Running Lattice simulations at large volumes and small quark masses gets extremely expensive, which is why we need supercomputers and months of computation time to get the configurations. The quark determinant in particular is numerically demanding to calculate due to its sheer size, which is at least as slow as the best LU-decomposition algorithm.

If one wants lighter quarks, the amount of statistics needed to suppress the statistical errors become very large,

and the computation times sky-rocket.

Lattice QCD: Challenges
The sign problem 1

Lattice QCD relies on Monte Carlo integration for the integral over link variables

$$Z = \int DU_\mu \det Q_{\text{uark}} e^{-S_{\text{gluon}}}$$

It only makes sense to use $\det Q_{\text{uark}} e^{-S_{\text{gluon}}}$ as a Monte Carlo weight if it is real
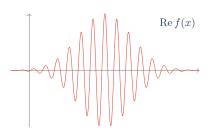
The second important limitation we want to look at for Lattice QCD is the so called "sign problem". It relates to the fact that without a baryon chemical potential, the fermion determinant is strictly real for all values of the gauge fields U. If we introduce a baryon chemical potential term to our lagrangian, $\mu \bar{\psi} \gamma_0 \psi$, the quark matrix gets complex values. Integrated over all configurations of U, the end result is of course real, so the imaginary components cancel out in the end. However, we sample the determinant with a Monte Carlo simulation, and thus getting these exact calculations is impossible. Also, it makes no sense to use $\det Q_{\text{uark}}$ as a probability if it is complex.

The link integral also suffer from exponensial cancellations

Example

$$f(x) = e^{-x^2 + i\theta x}$$

$\mathrm{Re}\, f(x)$

Lattice QCD: Challenges
The sign problem 2

$$f(x) = e^{-x^2 + i\theta x}$$
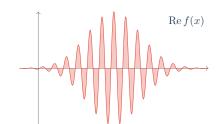
$\operatorname{Re} f(x)$
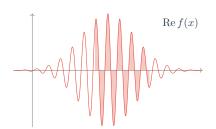
$$\int_{-\infty}^{\infty} dx\, f(x) = \sqrt{\pi}\, e^{-\frac{\theta^2}{4}}$$

Lattice QCD: Challenges
The sign problem 2

$$f(x) = e^{-x^2 + i\theta x}$$

$\text{Re}\, f(x)$

$\int_a^b \mathrm{d}x\, f(x)$ strongly depend on θ and $[a, b]$

Lattice QCD: Challenges
The sign problem 2

$f(x) = e^{-x^2 - i\theta x}$

$\mathfrak{Re}\, f(x)$

$\int_a^b dx\, f(x)$ strongly depend on θ and $[a, b]$

To demonstrate this point we have a classical example. Consider the function on the slide, which is an exponential with a complex phase. If we carry out the full integral, the imaginary parts of f all cancel out, and we are left with a real number. However the final result is exponentially suppressed by the frequency of the complex phase. On top of that, if we choose the boundaries in an unfortunate way, the final result will strongly depend on the boundaries. This is an issue as we in Lattice QCD do not have a strict control over our "boundaries" because the configurations are generated randomly.

The Effective Theory

Strong Coupling Expansion

Expansion around $\beta = \frac{2N_c}{g^2} = 0$

Recap

$$L_G \sim \beta \sum_{\mu,\nu} \text{tr } U_\mu(n) U_\nu(n+\mu) U_\mu^\dagger(n+\nu) U_\nu^\dagger(n)$$

This is an expansion in the number of plaquettes on the lattice

So the cost of putting one plaquette on the lattice is of the order β. If we take β to be small, we thus order by

order add one more plaquette to the lattice. The smallest non-zero contribution is gotten by adding 6 plaquettes

formed in a cube, but that only contributes to vacuum physics, so we aren't interested in that.

Hopping Parameter Expansion

One can rewrite the fermion matrix Q_{uark} as

$$Q_{\text{uark}}(x, y) = 1 - \kappa \sum_{\mu} \left(1 - \gamma_{\mu}\right) U_{\mu} \, \delta(x, y - \mu)$$
$$= 1 - \kappa H_{\text{op}}(x, y)$$

where $\kappa = \dfrac{1}{2(m_q + 4)}$
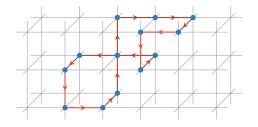
Hopping Parameter Expansion

And thus the fermion determinant $\det Q_{\text{uark}}$ as

$$\det Q_{\text{uark}} = \exp\left\{ -\sum_{n=1}^{\infty} \frac{1}{n} \kappa^n \operatorname{tr} H_{\text{op}}^n \right\}$$

Every H_{op} translates the quarks by one lattice spacing

Expansion around $\kappa = 0$ is an expansion in short range quark interactions

Hopping Parameter Expansion

And thus the fermion determinant $\det Q_{\text{quark}}$ as

$$\det Q_{\text{quark}} = \exp\left\{ -\sum_{n=1}^{\infty} \frac{1}{n} \kappa^n \operatorname{tr} H_{\text{op}}^n \right\}$$

Every H_{op} translates the quarks by one lattice spacing

Expansion around $\kappa = 0$ is an expansion in short range quark interactions

The $\operatorname{tr} H_{\text{op}}^n$ makes the fermion translate n lattice spacings. Because there is a trace, which also is a trace in space-time, the fermion has to hop in a loop. Because of the spin structure, a fermion cannot do any "backtracking". Meaning it cant hop forward then backward the same direction, simply because

$(1 + \gamma_\mu)(1 - \gamma_\mu) = 0.$

Hopping Parameter Expansion

Graphically, contributions to the expansion will be

- Closed loops
- No backtracking

The Effective Lattice Theory

Our goal

- Integrate out all spatial gauge links

$$\mathcal{Z} = \int DU_\mu \exp\left\{-S_{\text{action}}\right\}$$
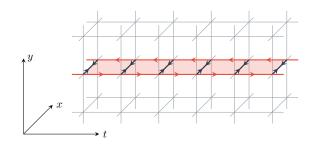
$$= \int DU_0 \exp\left\{-S_{\text{effective action}}\right\}$$
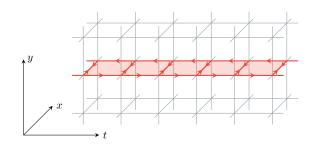
We create an effective action by carrying out some of the gauge link integrals by hand. Similar to how we got an effective action for the gluons by integrating out the fermions in the beginning, we get an effective action for the gauge links pointing in time direction by integrating out all the link pointing in spatial directions.
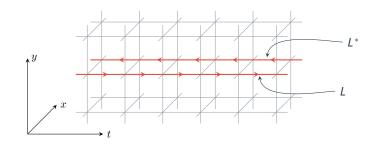
The reason we pick out the time direction specifically is of course because the time direction plays a special role

for Thermal Field Theories. One introduces temperature into a quantum field theory by compactifying the

temporal direction, meaning introducing period boundary-conditions, under which the fermions and bosons

transform in different ways.

The Effective Lattice Theory
Pure gluon contributions

Put a line of plaquettes in the time direction

The Effective Lattice Theory
Pure gluon contributions

Integrate over all spatial gauge links
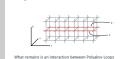
The Effective Lattice Theory
Pure gluon contributions

What remains is an interaction between Polyakov Loops

The Effective Lattice Theory
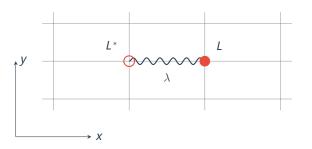Pure gluon contributions

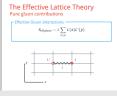What remains is an interaction between Polyakov Loops

As mentioned earlier, we are only interested in quantities that contribute to the thermodynamic of the system. For our system, that means quantities which span the full temporal direction, and thus picks up a temperature dependent component in the infinite volume limit.

For pure gauge action, in the strong coupling expansion, this means a plane of plaquettes spanning the full

temporal direction, as shown in the figure. We then integrate out the spatial links present in this strip of
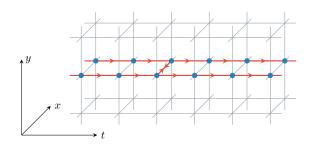
plaquettes, and are left with the Polyakov loops.

The Effective Lattice Theory
Pure gluon contributions

Effective Gluon Interactions

$$S_{\text{eff gluon}} \sim \lambda \sum_{\langle x,y \rangle} L(x) L^*(y)$$
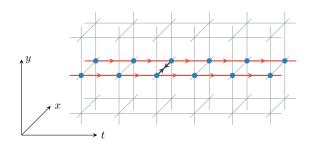
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The final result will thus be a nearest neighbour interaction between two Polyakov loops, or a continuos
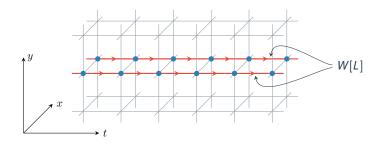
spin-system on a three dimensional lattice.

The Effective Lattice Theory
Pure quark contributions

Can produce a closed quark loop with multiple temporal windings

The Effective Lattice Theory
Pure quark contributions

Once again integrate out spatial links

The Effective Lattice Theory
Pure quark contributions
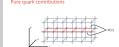
Producing an interaction between the *W* objects

For the fermions we are in very much the same situation. We need a quantity that spans the temporal direction of the lattice. The simplest such object is of course a single quark line, exclusively jumping in the temporal direction, going around the lattice. This is the contribution from static quarks, and this is of course included.
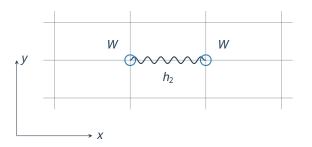
The next order term would be a quark that loops, jumps to a neighbouring site, loops, then jumps back, which is

the term depicted in the figure. Here again we integrate out the spatial links, and are left with the interaction of

two W-terms, the mathematical structure of which is not important for now.

The Effective Lattice Theory
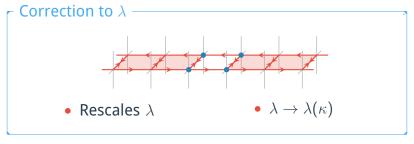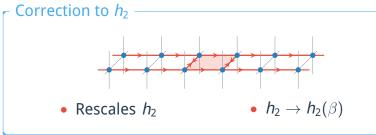## Pure quark contributions

Effective Gluon Interactions

$$S_{\text{eff quarks}} \sim h_2 \sum_{\langle x,y \rangle} W(x)W(y)$$

The Effective Lattice Theory
Mixed contributions

Correction to λ

- Rescales λ
- $\lambda \to \lambda(\kappa)$

Correction to h_2

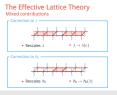- Rescales h_2
- $h_2 \to h_2(\beta)$

The Effective Lattice Theory
Mixed contributions

One can of course mix the terms from the two different expansions we are carrying out. Two examples of the possible terms can be seen in the figures. For these two simple cases, the mixing will only contribute as a shift in the nearest neighbour couplings, and can thus be absorbed by those.

There are higher order mixed terms that create entierly new interactions, but those are of much higher order of what we have shown here.

I will probably skip this slide.

The Effective Lattice Theory
Final form

The Effective Action

$$\mathcal{Z} = \int \prod_x \mathrm{d}L(x) \, \exp\left\{-S_{\text{eff action}}\right\}$$

$$S_{\text{eff action}} \sim \lambda \sum_{\langle x,y \rangle} L(x)L^*(y) + h_2 \sum_{\langle x,y \rangle} W(x)W(y)$$

Two options to proceed from here

1. Simulate the effective action
2. Analytically calculate it with a linked cluster expansion
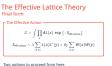
The Effective Lattice Theory
Final form

The Effective Action

$$\mathcal{Z} = \int \prod_x \mathrm{d}L(x)\, \exp\left\{-S_{\text{eff action}}\right\}$$

$$S_{\text{eff action}} \sim \lambda \sum_{\langle x,y \rangle} L(x)L^*(y) + h_2 \sum_{\langle x,y \rangle} W(x)W(y)$$

Two options to proceed from here

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The Effective Lattice Theory
Final form

─ The Effective Action ─────────

$$\mathcal{Z} = \int \prod_x \mathrm{d}L(x) \, \exp\left\{-S_{\text{eff action}}\right\}$$

$$S_{\text{eff action}} \sim \lambda \sum_{\langle x,y \rangle} L(x)L^*(y) + h_2 \sum_{\langle x,y \rangle} W(x)W(y)$$
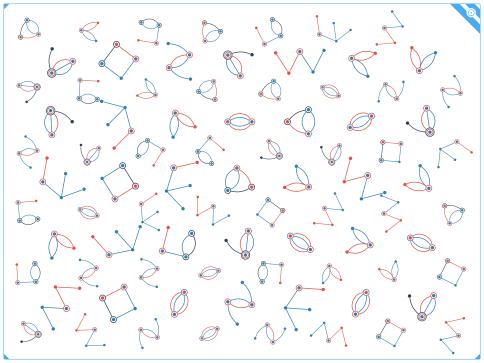
Two options to proceed from here
- Simulate the effective action
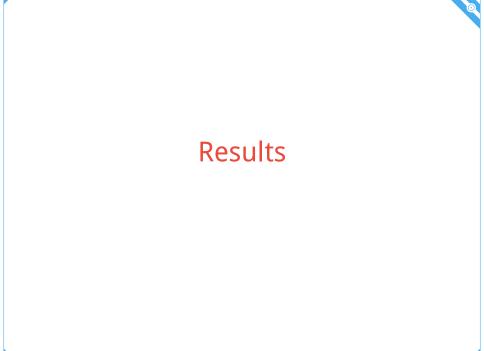- Analytically calculate it with a linked cluster expansion

Since the effective action still is in the exponential, it is impossible to carry out the integrals analytically, but we have significantly reduced the complexity of the system. The fermion determinant is no more, and we have also decreased the number of free parameters by orders of magnitude.

One way forward is to use the new action with a Monte Carlo simulation, which is what one of my colleage is doing. Another option would be to use a linked cluster expansion method to calculate the free energy from this analytically, and thus get expressions for baryon number density and other things analytically. This is the approach I have taken.
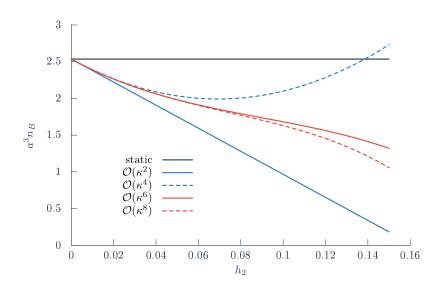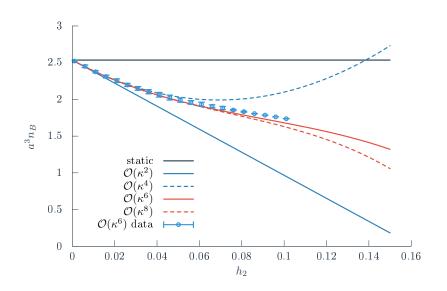
Simply a fun slide to make fun at what I put myself through to get the result analytically rather than numerically.
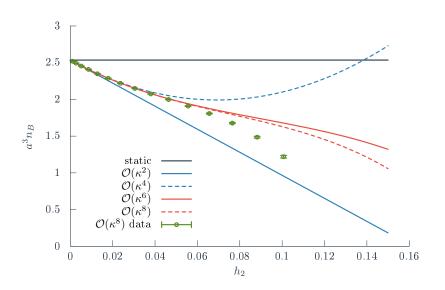
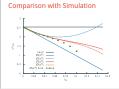# Results

Comparison with Simulation
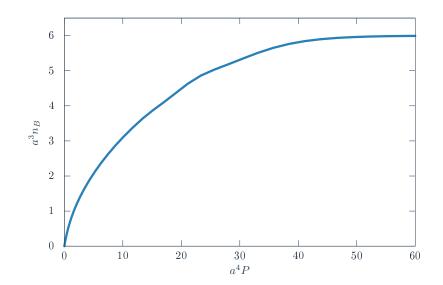
Comparison with Simulation
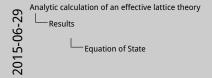
Comparison with Simulation

First of all see that it seems like the effective theory converges quite nicely as one systematically increases the order of h_2. When compared with simulations it also looks quite OK, however the κ^8 result seem to fail, but that might also be caused by the κ^6 just being a lucky hit. It should be noted that the error bars are actually way off, and do not represent the accuracy of the actual data, but are error bars for a certain element of the statistics carried out by the Monte Carlo algorithm. We are also having some numerical issues with simulating the effective theory at high order, so that might also disturb the results somewhat.

Equation of State

Analytic calculation of an effective lattice theory

└─ Results

   └─ Equation of State

If possible, I will try to get this plot in physical units rather than lattice units before my presentation.

Conclusion

Summary & Outlook

Summary

- Introduced two expansions for the lattice action
  - Strong coupling expansion
  - Hopping expansion

- Created a dimensionally reduced effective lattice theory

Summary & Outlook

Outlook

- Calculate higher order mixing terms

- Move more in the direction of the simulations

- ...

The project with the analytic evaluations is nearing its end as we have seen both its predictive power, but also its limitations when studying quantities such as the nucleon binding energy (not shown, but maybe I should). Although there exists method for higher order evaluations of the linked cluster expansion, we are not sure if the effort will be worth it in the end, and might leave it as a project that can be tied into the bigger picture at a later stage. Most of the talk has of course focused on the effective theory and not its analytic evaluation, which we will keep pursuing.