Lattice Monte Carlo Simulation with two Impurity worldlines

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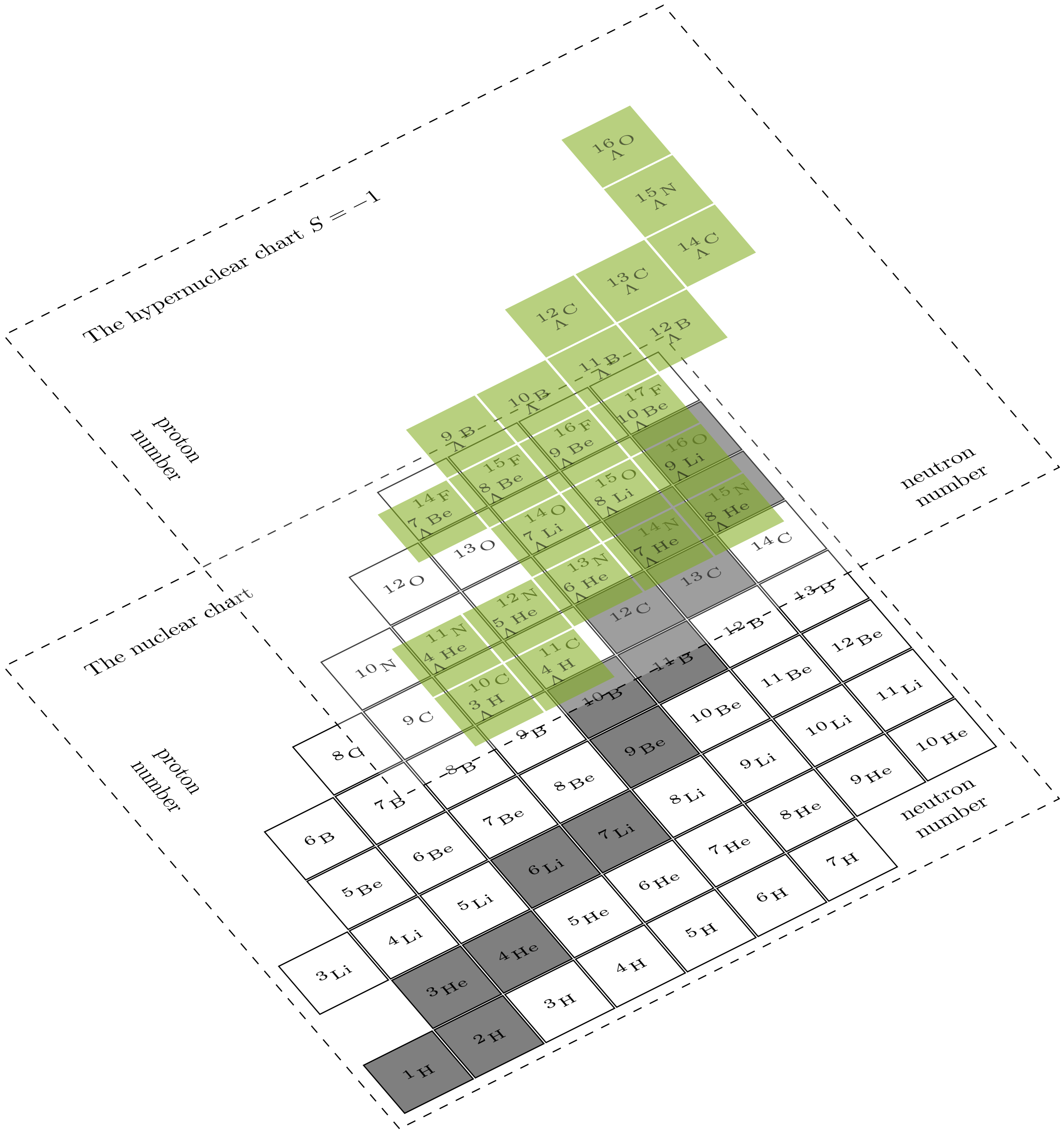
Outline

- Motivation > Connecting to my work in Darmstadt
- Our Setup and Method
  - Lattice Monte Carlo Methods
  - Nuclear Lattice Effective Field Theory
- Impurities as Worldlines
  - Results for two impurities
  - Where to go from here

Motivation

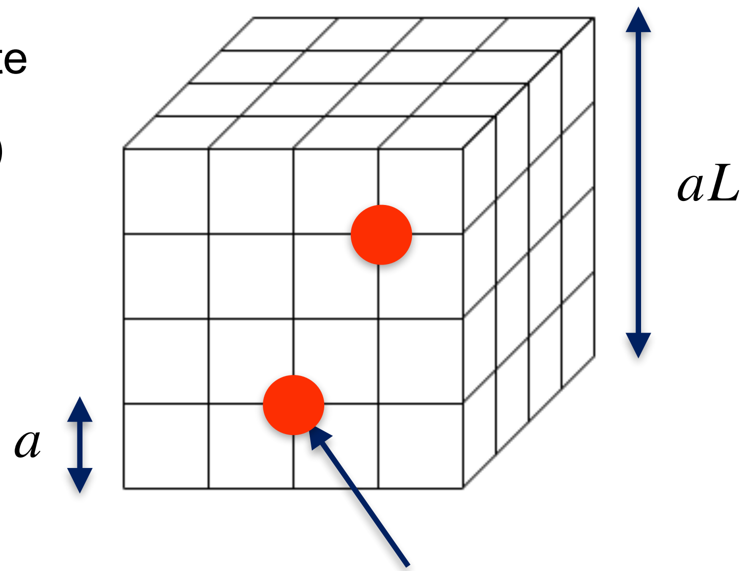
- Strangeness extends the nuclear Chart to a third dimension
- During my time in Darmstadt the focus was on three-body systems
- For heavier nuclei hyperons can be considered to be Impurities in a see of nucleons
- In principle the figure can be extended to a third $S = -2$ Layer
- Ξ and $\Lambda\Lambda$ hyerpernuclei



Method: Lattice Monte Carlo

- Lattice ⇒ Cubic Volume of size $(La)^3$ with discrete lattice site
  (a = lattice spacing, serves as UV cutoff for the EFT $\Lambda = \frac{\pi}{a}$)

- We need to make our Hamiltonian discrete.



Example: Spin ↑ particle(s)

$$H = \frac{1}{2m}\int \mathrm{d}^3 r\, \nabla a^\dagger(\boldsymbol{r}) \cdot \nabla a(\boldsymbol{r}) = -\frac{1}{2m}\int \mathrm{d}^3 r\, a^\dagger(\boldsymbol{r}) \cdot \nabla^2 a(\boldsymbol{r})$$

$\Rightarrow$

Nearest neighbours

$$H_L = \frac{3}{\tilde{m}}\sum_{n} a_i^\dagger(\boldsymbol{n}) a_i(\boldsymbol{n}) - \frac{1}{2\tilde{m}}\sum_{n}\sum_{l=1}^{3}\left[a_i^\dagger(\boldsymbol{n}) a_i(\boldsymbol{n}+\hat{\boldsymbol{e}}_l) + a_i^\dagger(\boldsymbol{n}) a_i(\boldsymbol{n}-\hat{\boldsymbol{e}}_l)\right]$$

simplest version, many more possible, do the same with the potential

Method: Lattice Monte Carlo II

- We want to calculate the (binding) energy of a system

- Typical Idea, consider partition function:

$$\mathcal{Z} = \mathrm{Tr}\left(\exp(-\beta H)\right)$$

- Remember TheoV/QFT2/ path integral seminar
- express this in terms of a Grassmann path integral

$$\mathcal{Z} = \int \left[\prod_{\boldsymbol{n},n_t} \mathrm{d}\xi(\boldsymbol{n},n_t)\mathrm{d}\xi^*(\boldsymbol{n},n_t) \right] \exp(-S[\xi,\xi^*]) \simeq \mathrm{Tr}(M^{N_t}) + \ldots$$

- Where M is the normal ordered transfer matrix operator for one time step
- Define now a trial state $|\Psi_T(t')>$ and the Euclidean time projection amplitude

$$Z(t) = \langle \Psi_T(t') | \exp(-Ht) | \Psi_T(t') \rangle$$

- Define assigned energy in the usual way $E(t) = -\partial_t Z(t) \quad t \to \infty$
- Obtain energy of the lowest eigenstate of H with a non-vanishing overlap with the trial state

Method: Lattice Monte Carlo III

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- For a general Operator $\mathcal{O}$, the expectation value in path integral formalism is given

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}s \; \mathcal{O}[s] \exp(-S_E[s, \beta])$$

$$\langle \mathcal{O} \rangle = \approx \frac{\sum_s \mathcal{D}s \; \mathcal{O}[s] \exp(-S_E[s])}{\sum_s \exp(-S_E[s])}$$ $\propto$ complex phase $\Rightarrow$ sign proplem

Metropolis Accept/Reject sampling with respect to the action
(Importance Samling, Markov chains …)

- Auxiliary Fields to handle many particles efficiently:
- Idea: Replace Interactions between nucleons with
  Interaction of a nucleon with an auxiliary field

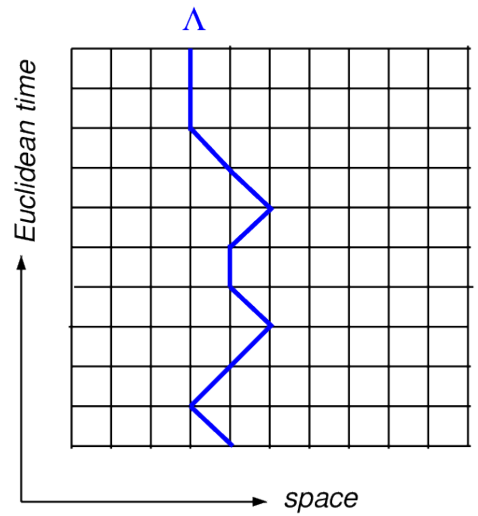
$$\exp(-\frac{C}{2}(N^\dagger N)^2) = \sqrt{\frac{1}{2}} \int \mathrm{d}A \exp\left[-\frac{A^2}{2} + \sqrt{C} A (N^\dagger N)\right]$$

Since Nucleons only interact with an auxiliary field $\Rightarrow$ Perfect for parallel computing

Mitglied der Helmholtz-Gemeinschaft

Nuclear Lattice Effective field theory

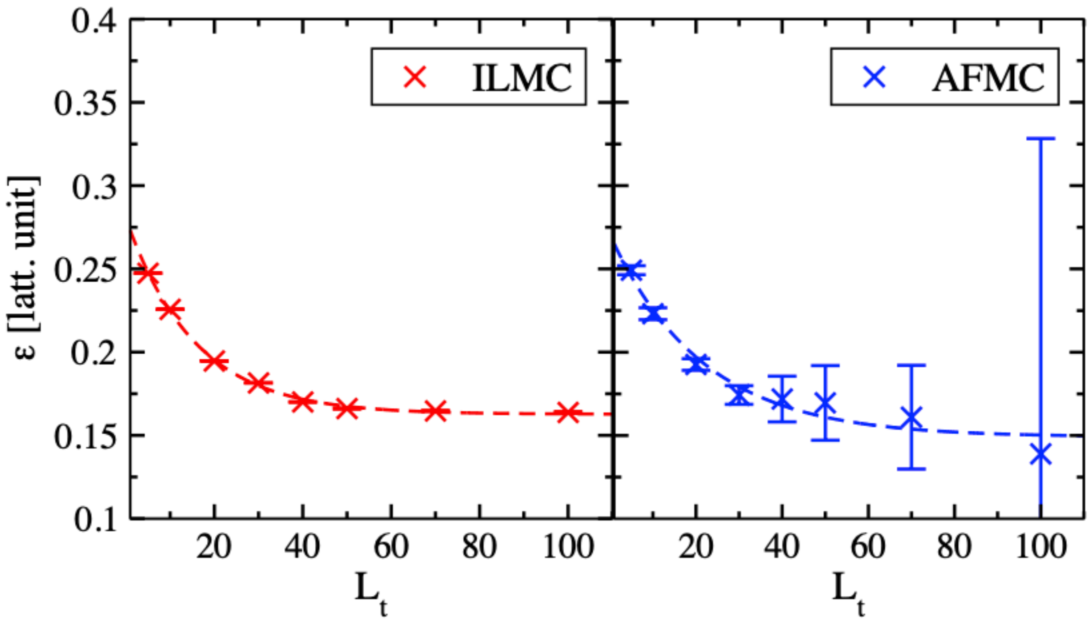
- Use Chiral Effective field theory to construct forces between nuclei
- Allows Calculation of energies and matter radii of nuclei
- Addition of Hyperons is an additional challenge, since AFMC does not converge as good as in a pure nuclear matter simulation



(D. Frame, T. A. Lähde, D. Lee, U.-G. Meißner)

Need to develop a method that threats this impurities more efficient
Treat Impurity as worldline:

(S.Bour, D.Lee, H.-W. Hammer, U.-G. Meißner)



We however want to study systems with more impurities !!

$$\hat{H}_0 = \frac{1}{2m} \sum_{s=\uparrow_a,\uparrow_b,\downarrow} \int \mathrm{d}^3\boldsymbol{r}\, \nabla a_s^\dagger(\boldsymbol{r}) \nabla a_s(\boldsymbol{r})$$

← Kinetic Energy Term

$$\hat{H}_I = C_{II} \int \mathrm{d}^3\boldsymbol{r}\, \hat{\rho}_{\uparrow_b}(\boldsymbol{r})\hat{\rho}_{\uparrow_a}(\boldsymbol{r}) + C_{IB} \int \mathrm{d}^3\boldsymbol{r} \left[\hat{\rho}_{\uparrow_a}(\boldsymbol{r})\hat{\rho}_{\downarrow}(\boldsymbol{r}) + \hat{\rho}_{\uparrow_b}(\boldsymbol{r})\hat{\rho}_{\downarrow}(\boldsymbol{r})\right]$$

← Contact Interactions

Worldline - Worldline Interaction

Worldline - Background Interaction

Idea: Integrate out the impurities from the lattice action :

$$\langle \chi_{n_{t+1}}^{\downarrow}, \chi_{n_{t+1}}^{\uparrow_a}, \chi_{n_{t+1}}^{\uparrow_b} | \hat{M} | \chi_{n_t}^{\downarrow}, \chi_{n_t}^{\uparrow_a}, \chi_{n_t}^{\uparrow_b} \rangle \Rightarrow \langle \chi_{n_{t+1}}^{\downarrow} | \hat{\tilde{M}} | \chi_{n_t}^{\downarrow} \rangle$$

With any state in occupation number basis is given by:

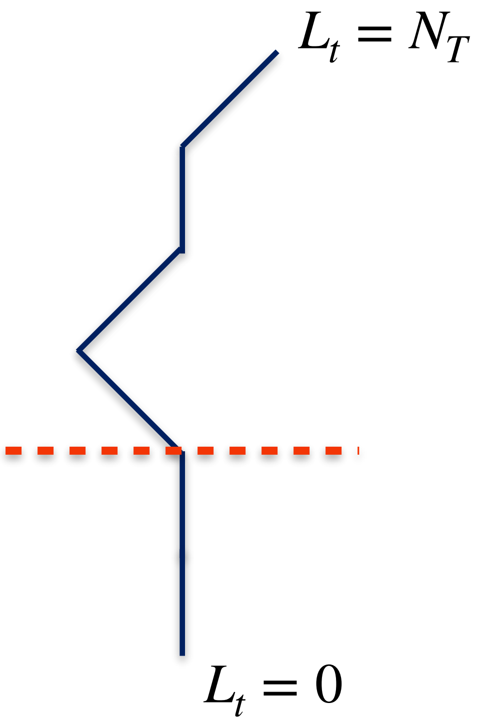
$$|\chi_{n_t}^{\downarrow}, \chi_{n_t}^{\uparrow_a}, \chi_{n_t}^{\uparrow_b}\rangle = \prod_{\boldsymbol{n}} \left[a_{\downarrow}^{\dagger}(\boldsymbol{n})\right]^{\chi_{n_t}^{\downarrow}(\boldsymbol{n})} \left[a_{\uparrow_a}^{\dagger}(\boldsymbol{n})\right]^{\chi_{n_t}^{\uparrow_a}(\boldsymbol{n})} \left[a_{\uparrow_b}^{\dagger}(\boldsymbol{n})\right]^{\chi_{n_t}^{\uparrow_b}(\boldsymbol{n})} |0\rangle$$

- Naive way: Generate random worldlines ⇒ Low acceptance Rate

  ↘ Long calculations

What we want:

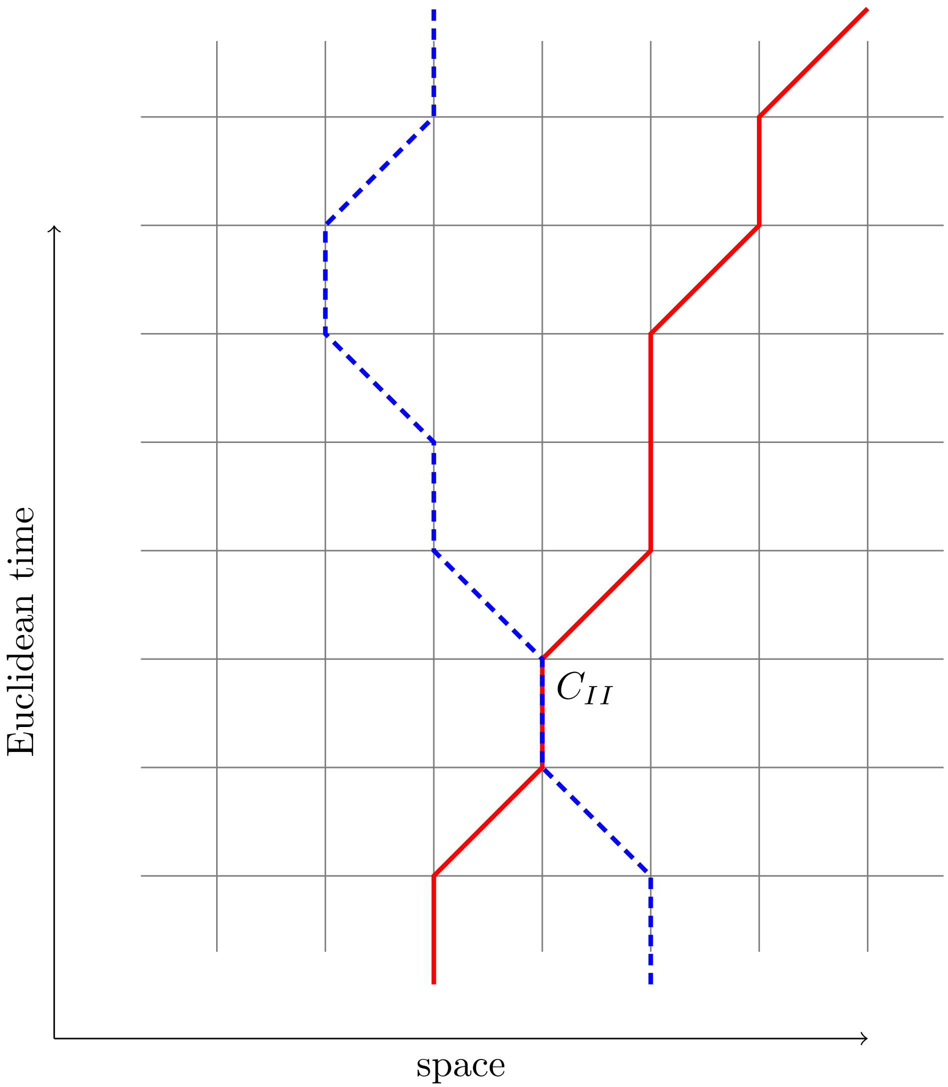
Worldlines that are likely to be accepted,
But also cover the configuration space quickly



- Randomly cut one worldline into two pieces update only one part!
- Likelihood for acceptance increases
- Experience: Most Contributions come from Worldlines that do not hop often

  ↘ Shorter calculations

What can happen?



- both worldline hop

$$\overline{M}^{\boldsymbol{n}\pm\hat{l},\boldsymbol{n}}_{\boldsymbol{n}'\pm\hat{l}',\boldsymbol{n}'} = W_h^2 : e^{-\alpha H_0^{\downarrow}} :$$

- one worldline hops, one stays

$$\overline{M}^{\boldsymbol{n}\pm\hat{l},\boldsymbol{n}}_{\boldsymbol{n}',\boldsymbol{n}'} = W_h W_s : e^{-\alpha H_0^{\downarrow} - \frac{\alpha C_{IB}\,\rho_\downarrow(\boldsymbol{n}')}{W_s}} :$$

- both worldlines stay

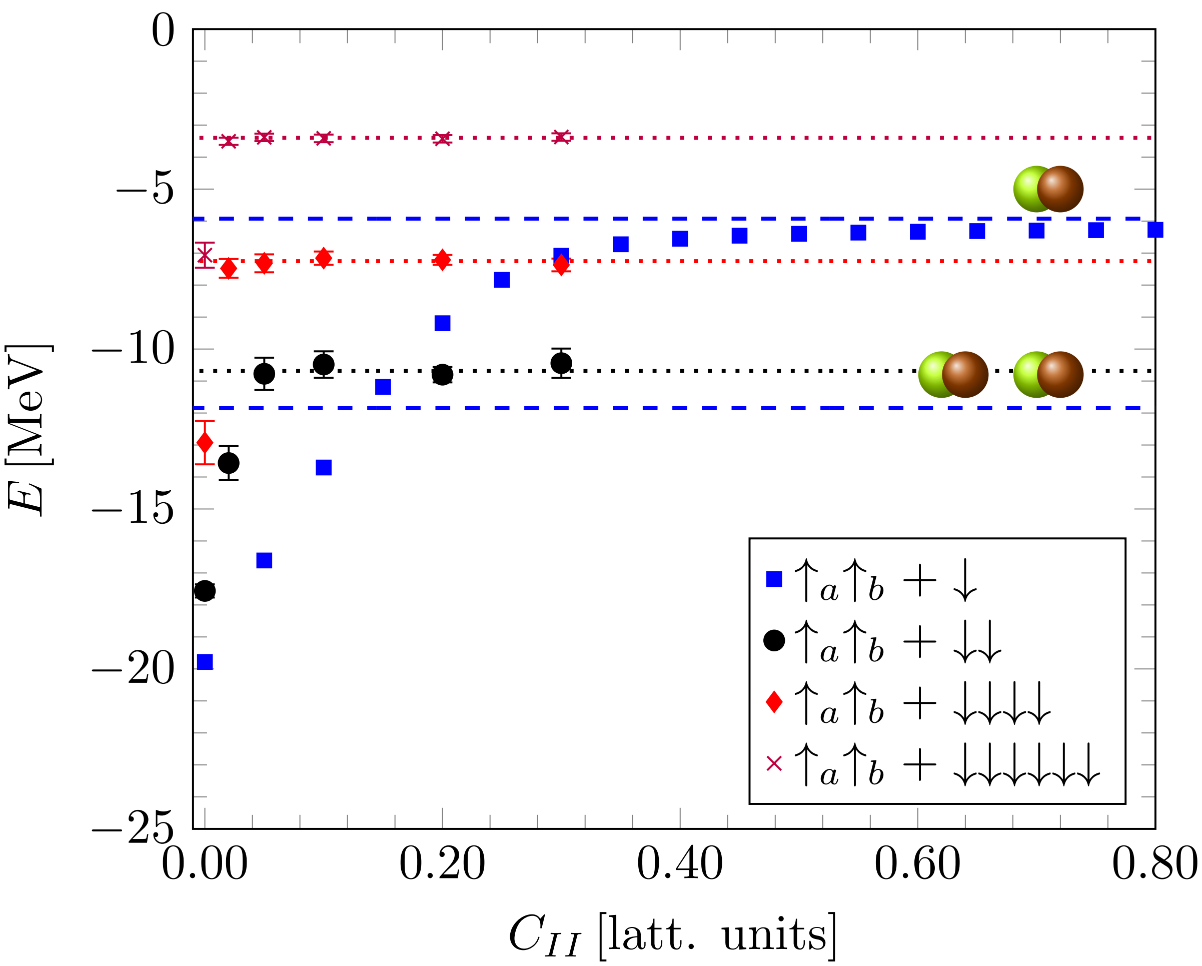
$$\overline{M}^{\boldsymbol{n},\boldsymbol{n}}_{\boldsymbol{n}',\boldsymbol{n}'} = W_s^2 : e^{-\alpha H_0^{\downarrow}} \exp\left[\frac{-\delta_{\boldsymbol{n},\boldsymbol{n}'}\alpha C_{II}}{W_s^2} - \frac{\alpha C_{IB}\rho_\downarrow(\boldsymbol{n})}{W_s} - \frac{\alpha C_{IB}\,\rho_\downarrow(\boldsymbol{n}')}{W_s} + \mathcal{O}(\alpha^2)\right] :$$

Summary : How does the Interaction work:

- Worldline only interacts with the background particles if it stays on the same lattice site $\boldsymbol{n}$ from one timeslice to the next one
- Interaction happens on the lattice side $\boldsymbol{n}$
- If both Worldlines stay on the same lattice side $\boldsymbol{n}$ an additional contact interaction between the two impurities is felt by the whole lattice

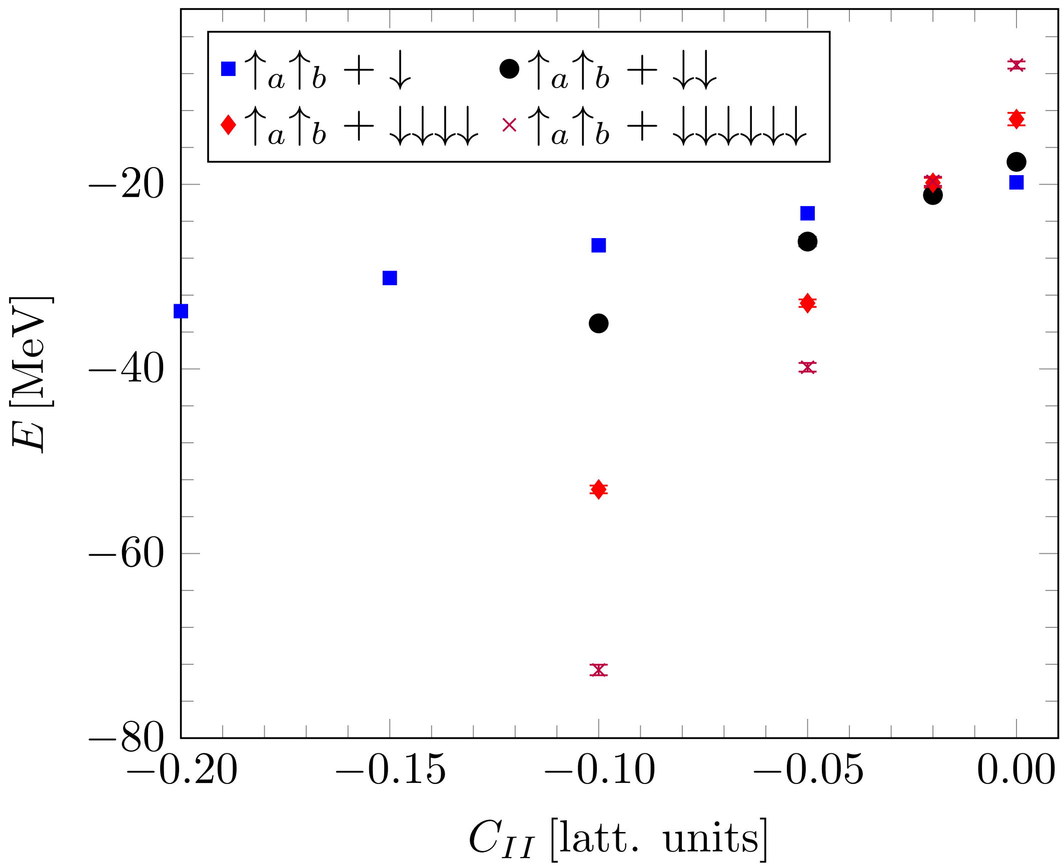
$$\overline{M}^{\boldsymbol{n},\boldsymbol{n}}_{\boldsymbol{n}',\boldsymbol{n}'} = W_s^2 : e^{-\alpha H_0^{\downarrow}} \exp\left[\frac{-\delta_{\boldsymbol{n},\boldsymbol{n}'}\alpha C_{II}}{W_s^2} - \frac{\alpha C_{IB}\rho_{\downarrow}(\boldsymbol{n})}{W_s} - \frac{\alpha C_{IB}\,\rho_{\downarrow}(\boldsymbol{n}')}{W_s} + \mathcal{O}(\alpha^2)\right] :$$

Results: Attractive Impurity-Background Interaction
Repulsive Impurity-Impurity interaction



- Impurity-Background interaction chosen to be attractive $a \sim 3$ fm
- Trimer stays bound even for very repulsive C_{II}
- The four particle bound state however consists out of two dimers
- Further particles fill up the fermi sea of the box and do not contribute to the binding

Results: Attractive Impurity-Background Interaction
Attractive Impurity-Impurity interaction



- Around $C_{II} \sim -0.02$ the four particle system is deeper bound than the 3-body system
- Higher-particle systems show a similar behaviour at the same point
- Indication of a rich phase structure

Summary and Outlook

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- Impurity Monte Carlo offers a powerful tool to add one or more Impurities on top of a nuclear lattice effective field theory simulation
- Offers application in different fields as well, such as atomic physics …
- So far only applied for non-interacting background
- Combine with full NLEFT code to tackle double Λ hypernuclei