Nuclear Lattice Effective Field Theory

— *Code Strategy Meeting*

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Intention of the Meeting

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Code Demonstration

- Simplified physical / mathematical background
- Idea for numerical implementation

Demands

- What are the numerical dimensions intended to analyze?
- Which features need to be *flexible?*

Strategy / Discussion (C++)

- Strategy for **parallelization** of code
- Ideas for further **optimization**

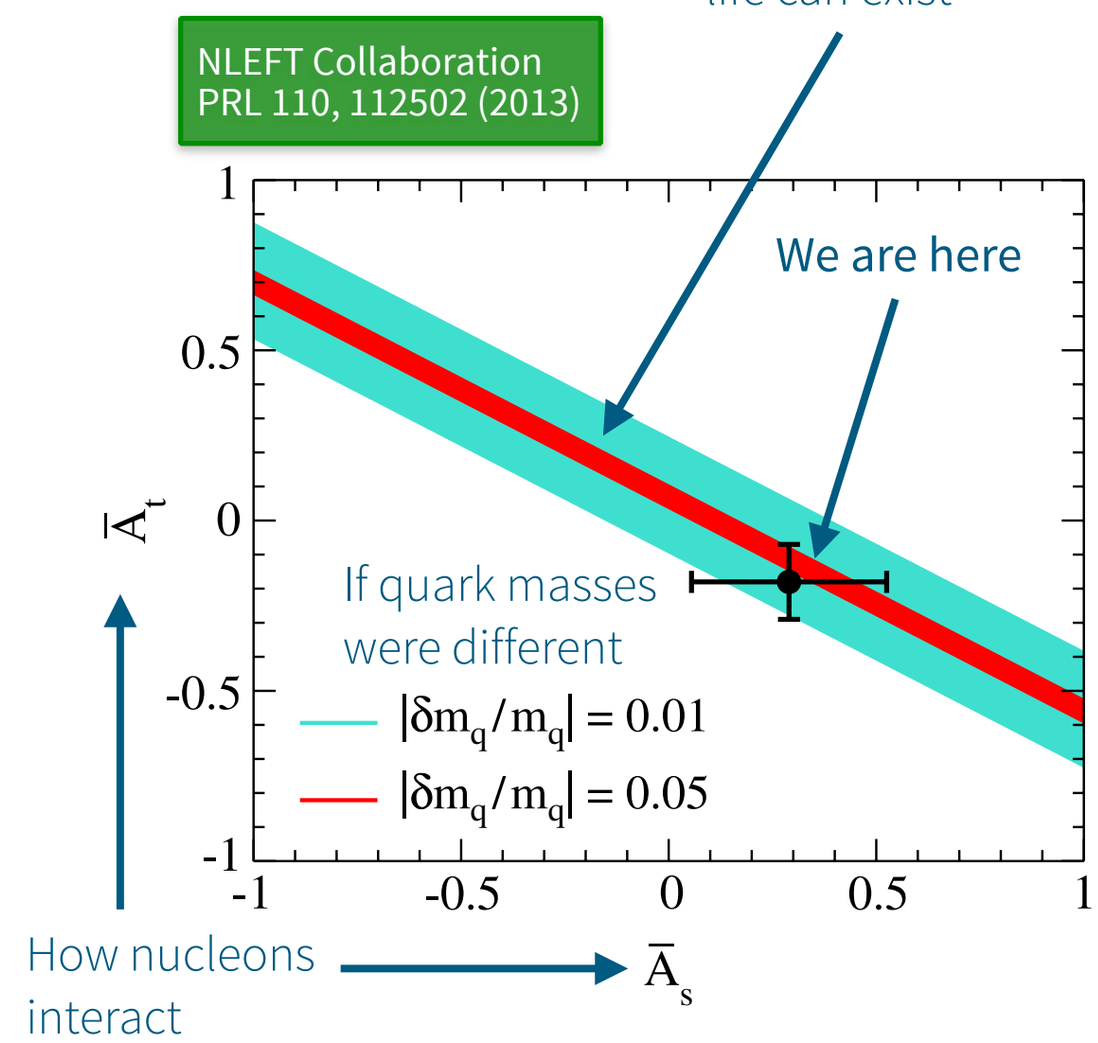
Current Algorithm

Nuclear Lattice Effective Field Theory

- ‘ab initio’ description of nuclear cores
  — From protons and neutrons to heavy nuclei
- **Compute binding energies and excitation levels**
  — Anthropic Principle: the Hoyle State

Future Ideas

- **Connection to new physics**
  — Help in finding Dark Matter candidates? (My PhD thesis)
- **Description of non-nuclear systems**
  — Tool to access general many-body quantum systems



Path Integral

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(tree - 222171)
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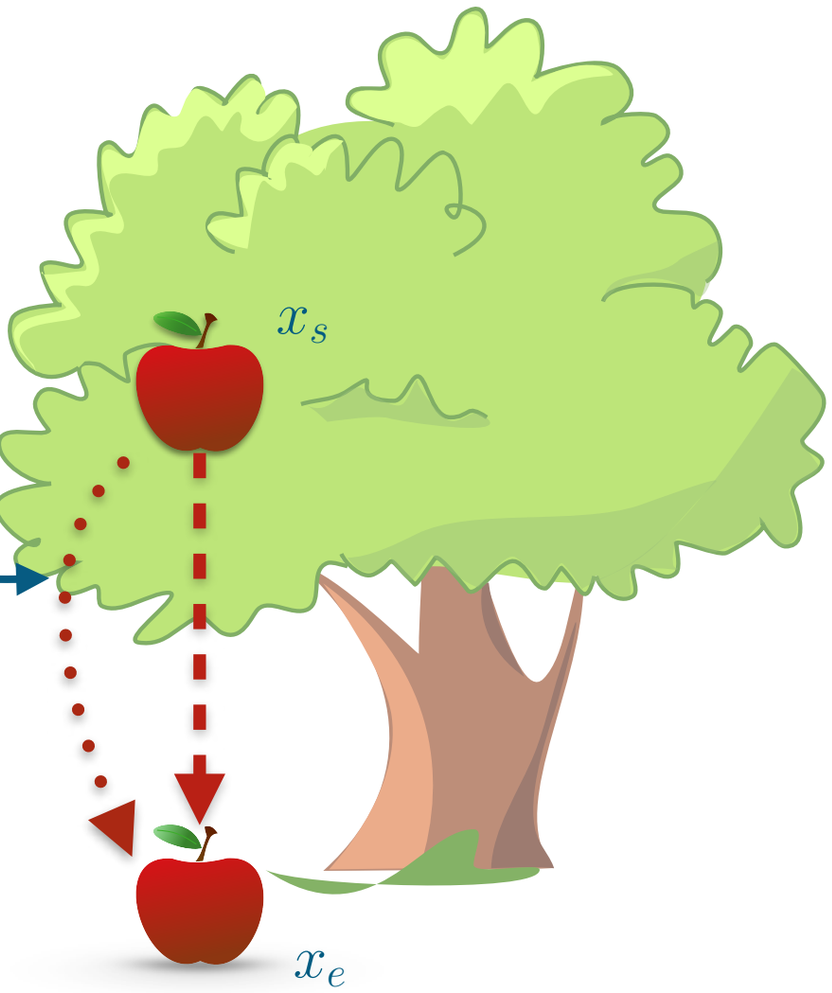
‘Classical’ World

- Classically object follows deterministic path
  - ➡ Classical path corresponds to extremal action

$$x_0(t) \rightarrow S[x_0(t)] \leq S[x(t)]$$

$$x(t_s) = x_s\,, \quad x(t_e) = x_e$$



‘Quantum’ World

- Object follows all possible paths (weighted)
  - ➡ Quantum paths are associated with a probability

$$\langle x_s \rightarrow x_e \rangle = \int \mathsf{D}[x(t)]\, e^{-S_E[x(t)]}$$

integration over all possible paths

Probability of path

Computationally

- Path integral can be expanded in eigenstates corresponding to energy

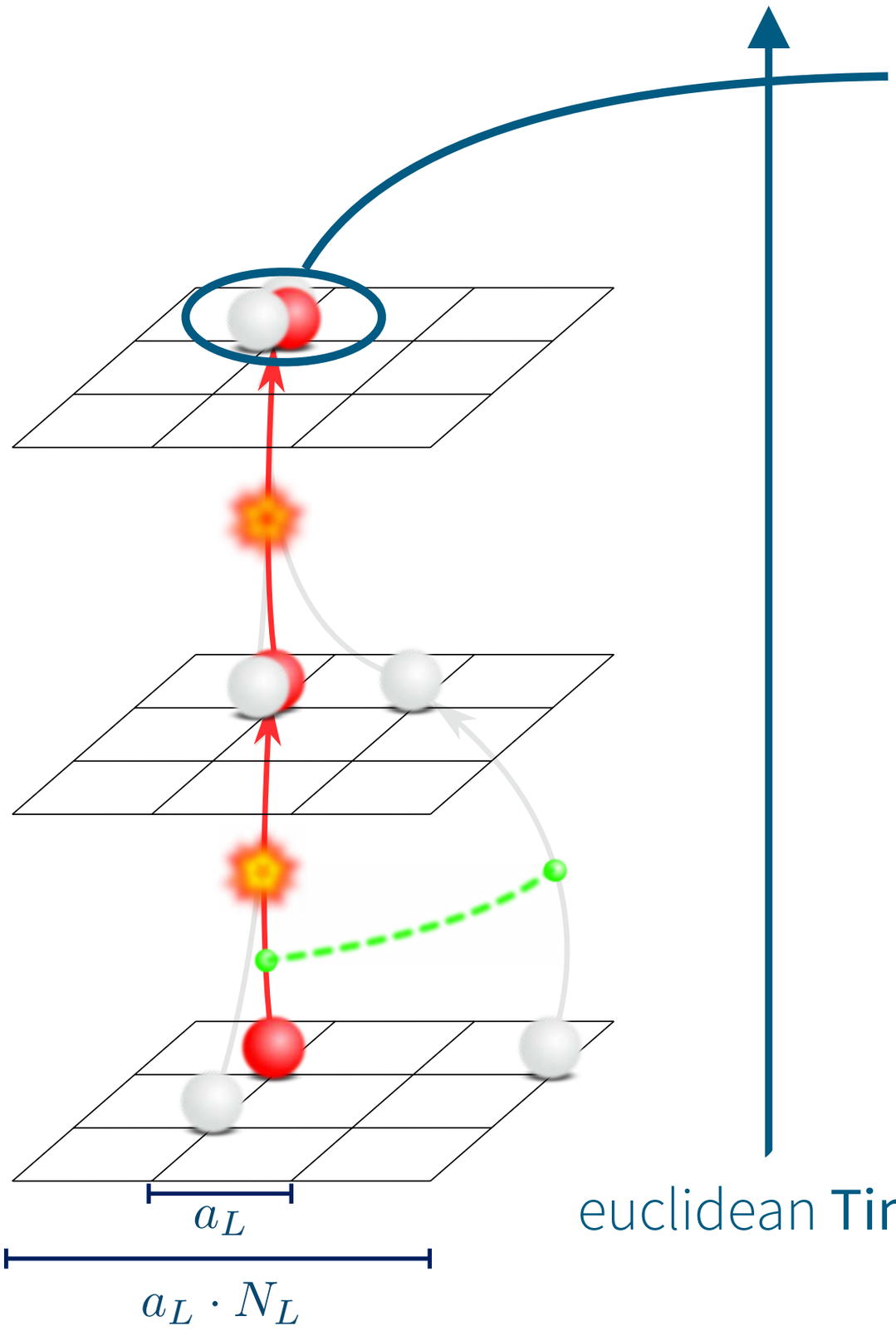
$$\int \mathsf{D}[x(t)]\, e^{-S_E[x(t)]} = |\, c_0\,|^2\, e^{-E_0(t_e - t_s)} + |\, c_1\,|^2\, e^{-E_1(t_e - t_s)} + \cdots$$

- Path integral can be expressed by transfer matrix (non-relativistic)

$$\int \mathsf{D}[x(t)]\, e^{-S_E[x(t)]} = \mathsf{Tr}\left[\, \mathcal{M}^{N_T}\,\right] \qquad N_T = \frac{t_e - t_s}{a_T}$$

temporal lattice spacing

The Rough Idea



Measurement

- Insert and extract structures of interest

Convergence

- Path of highest probability leads to state of minimal energy: nuclear core

Evolution

- Nucleons propagate through space
- Possible paths have different probabilities

Initialization

- Place individual nucleon on lattice (wave function)

Naive Approach

— Example case for two particles

Normal ordering: can only connect to particle once

Tri- or more diagonal in vector space

Transfertmatrix

$$\mathcal{M} = :\exp\{-a_t\,(T+V)\}: = \left(\mathbb{1} - a_t(T_1+T_2+V_{12}) + a_t^2 T_1 T_2\right)$$

- Obtain solutions by solving for eigenvalues or applying as projector

$$\mathcal{M}^{N_T}\cdot|\Psi\rangle = e^{-E_0\,a_T N_T}\,|\Psi^0\rangle + e^{-E_1\,a_T N_T}\,|\Psi^1\rangle + \cdots$$

Antisymmetric in exchange

Scaling not feasible for many particle state!

Basis

- Each particle lives in 3-dimensional space $|\Psi\rangle = |\vec{\psi}_1, \vec{\psi}_2\rangle \in 4N_L^3 \cdot 4N_L^3$

Proton, neutron, spin up and down

Application of Transfer matrix

- Transfer matrix has coupled and uncoupled parts

$$\mathcal{M}\cdot|\vec{\psi}_1,\vec{\psi}_2\rangle = |\vec{\psi}_1,\vec{\psi}_2\rangle - a_t\,|T_1(\vec{\psi}_1),\vec{\psi}_2\rangle - a_t\,|\vec{\psi}_1,T_2(\vec{\psi}_2)\rangle + a_t^2\,|T_1(\vec{\psi}_1),T_2(\vec{\psi}_2)\rangle - a_t\,|V_{12}(\vec{\psi}_1,\vec{\psi}_2)\rangle$$

Structures independent on 'other' particle

Coupled structure

HMC Approach

— HMC Update

Quantity of Interest

¥ Want to compute partition function

$$\mathcal{Z}(N_T) := \langle \phi_1, \phi_2 | \mathcal{M}^{N_T} | \phi_1, \phi_2 \rangle \qquad \langle \phi_1, \phi_2 | \phi_1, \phi_2 \rangle = \det \begin{pmatrix} \langle \phi_1 | \phi_1 \rangle & \langle \phi_1 | \phi_2 \rangle \\ \langle \phi_2 | \phi_1 \rangle & \langle \phi_2 | \phi_2 \rangle \end{pmatrix}$$

Auxiliary Field Integration

¥ Determinant in presence of auxiliary field (complex for each individual field)

$$Z(N_T) = \sum_{[s(n_t)]} \det \begin{pmatrix} \langle \phi_1 | M[s(N_T)] \cdots M[s(1)] | \phi_1 \rangle & \langle \phi_1 | M[s(N_T)] \cdots M[s(1)] | \phi_2 \rangle \\ \langle \phi_2 | M[s(N_T)] \cdots M[s(1)] | \phi_1 \rangle & \langle \phi_2 | M[s(N_T)] \cdots M[s(1)] | \phi_2 \rangle \end{pmatrix}^{\#} =: \sum_{[s(n_t)]} \det(1 + A[s(n_t)])$$

¥ Using Monte Carlo integration

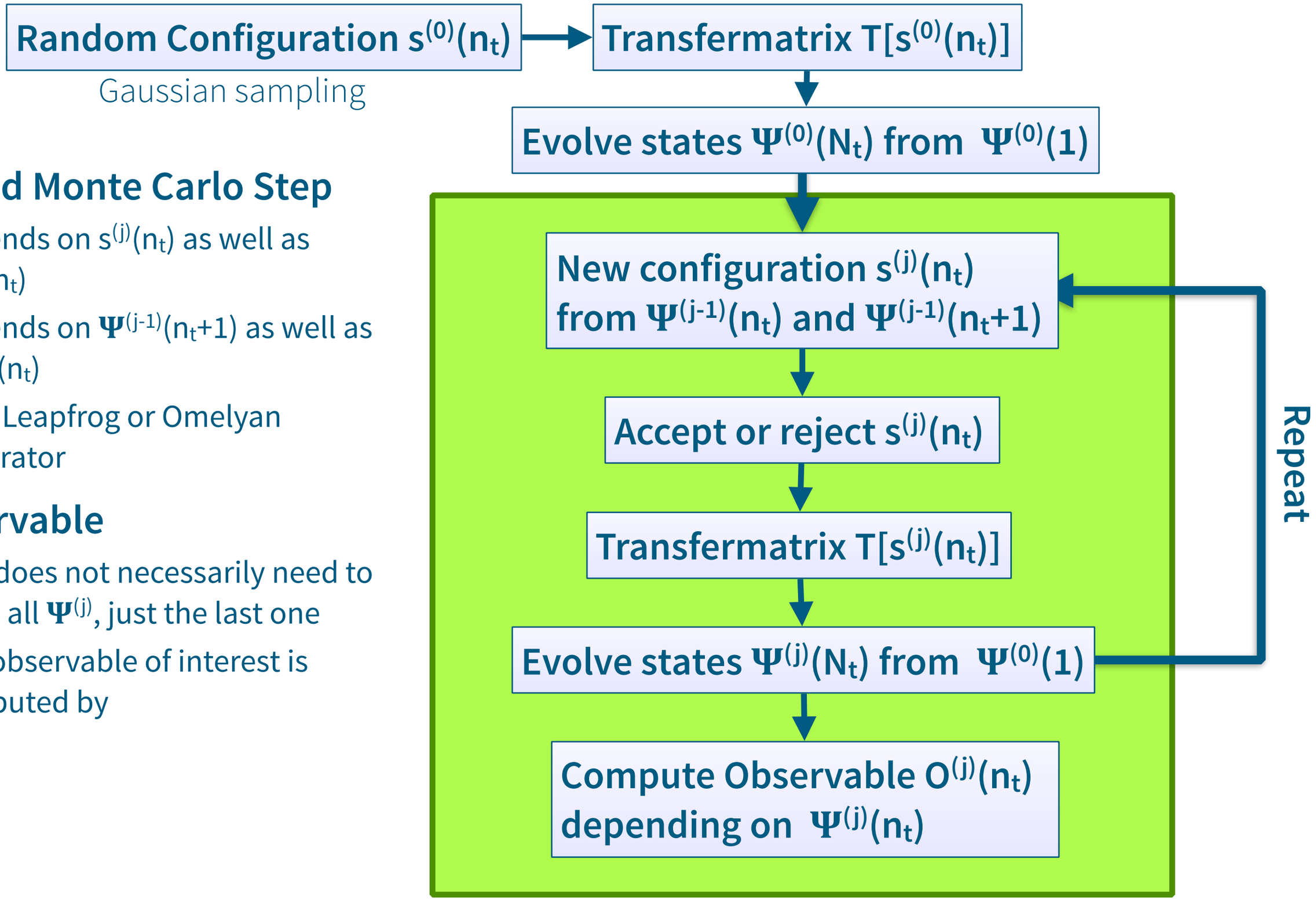
$$\frac{1}{N_c} \sum_{n_c=1}^{N_c} \exp\left(-i\phi\left[\vec{s}^{(n_c)}(n_t)\right]\right)^{\#} \approx \frac{1}{N_c} Z(N_T) \qquad P[\vec{s}(n_t)] = \left| \det(1 + A[\vec{s}(n_t)]) \right|$$

¥ Sampling of auxiliary field distribution depends on states at two time-slic

$$s^{(n_c+1)}(n_t) = s^{(n_c)}(n_t) + \#p(s_i^{(n_c)}(n_t+1), s_i^{(n_c)}(n_t))$$

New Code Design

— Workflow



Hybrid Monte Carlo Step

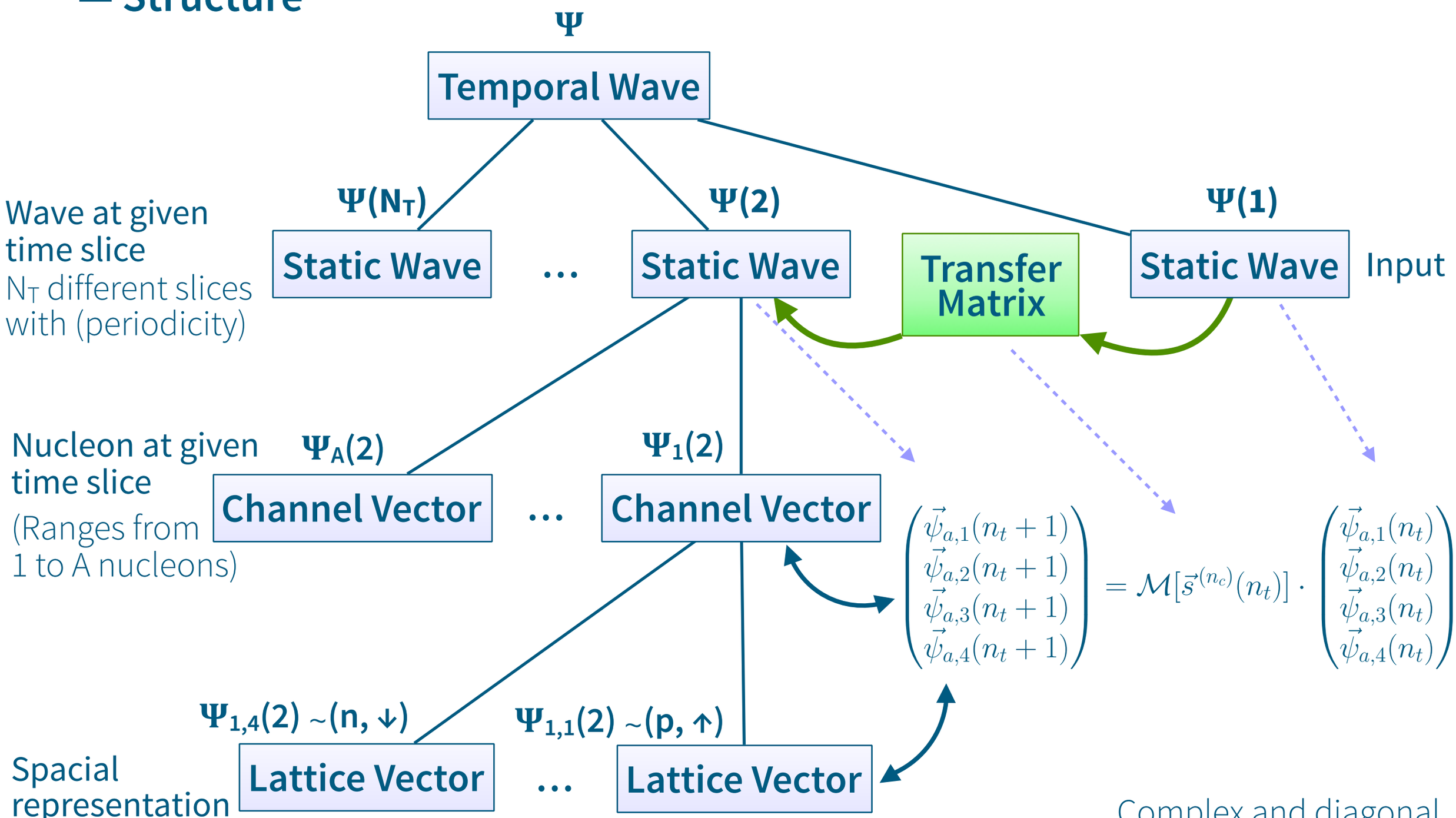
- Depends on $s^{(j)}(n_t)$ as well as $s^{(j-1)}(n_t)$
- Depends on $\Psi^{(j-1)}(n_t+1)$ as well as $\Psi^{(j-1)}(n_t)$
- Uses Leapfrog or Omelyan integrator

Observable

- One does not necessarily need to store all $\Psi^{(j)}$, just the last one
- The observable of interest is computed by

New Code Design

— Structure



New Code Design

— Demands

Dimensionality

- Temporal dimension
  - For reasonable extraction $N_T \approx 12+$
- Spacial dimension
  - Lattice spacing dependence of interest
  - $N_L \approx 30+$ desireable
- Number of HMC trajectories
  - Depends on observable
  - Similar algorithms use order $N_C > 10^6$ configurations
- Number of nucleons
  - Light P-Shell nuclei of interest $A < 20$
  - Some experiments use $A \approx 130$

Functionality

- **Scalability** in different dimensions
  - Importance supposingly: $N_C > A > N_T > N_L$
- Sufficiently **modularized** / easily **exchangeable structures**
  - Different operator structures specifically in transfer matrix are of interest
- Easy to use / **Pseudocode like** interface on production level
  - Specific purpose: uncertainty analysis and usability