Nuclear Lattice Simulations

Lecture 3: Chiral Effective Field Theory on the Lattice

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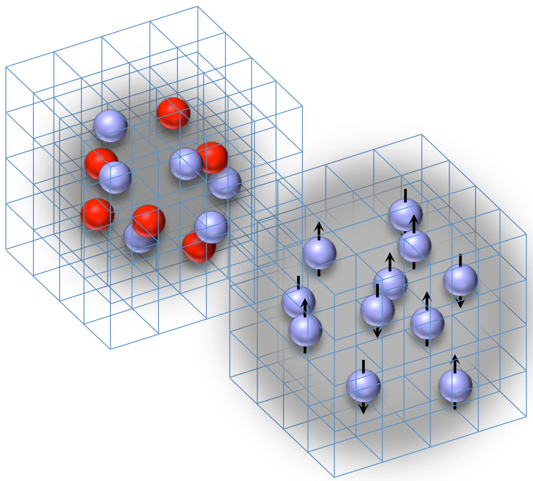

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Lectures

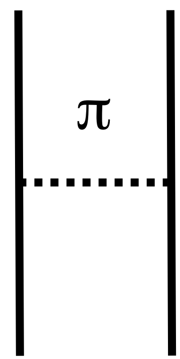
Lecture 1: Lattice Field Theory and Monte Carlo Methods

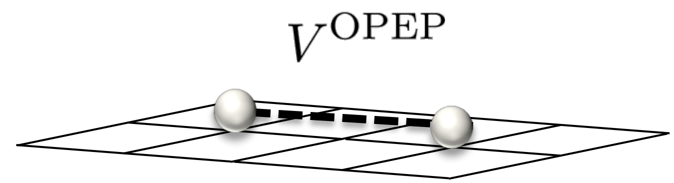
Lecture 2: Path Integrals, Transfer Matrices, and Auxiliary Fields

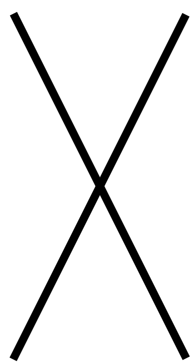
Lecture 3: Chiral Effective Field Theory on the Lattice

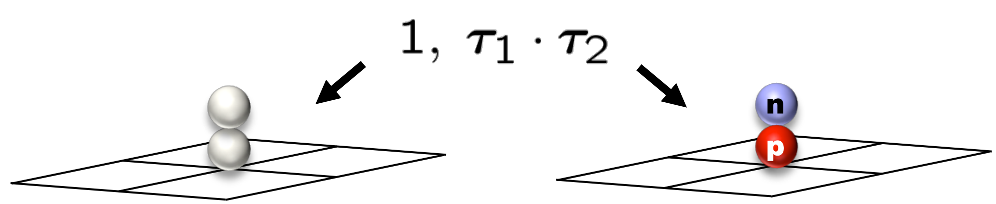
Lecture 4: Applications of Nuclear Lattice Simulations

Leading order interactions



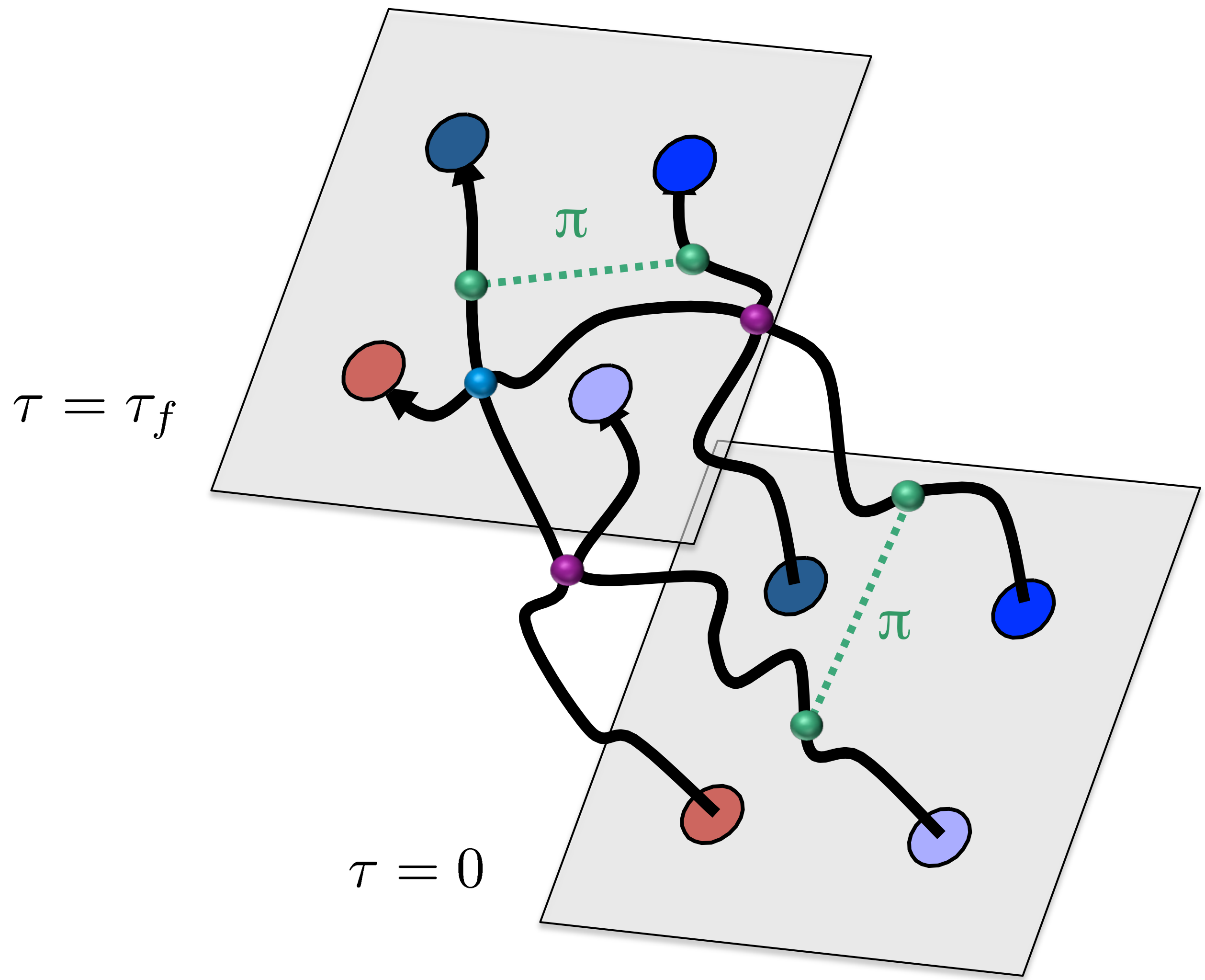






$+$ other interactions depending on chiral effective field theory expansion

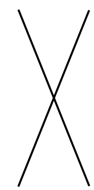
$$\exp(-H\tau) =: \exp(-H\Delta t) : \cdots : \exp(-H\Delta t) :$$



Auxiliary field method

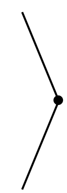
We write exponentials of the interaction using a Gaussian integral identity

$$:\exp\left[-\frac{C\Delta t}{2}(N^{\dagger}N)^{2}\right]:$$



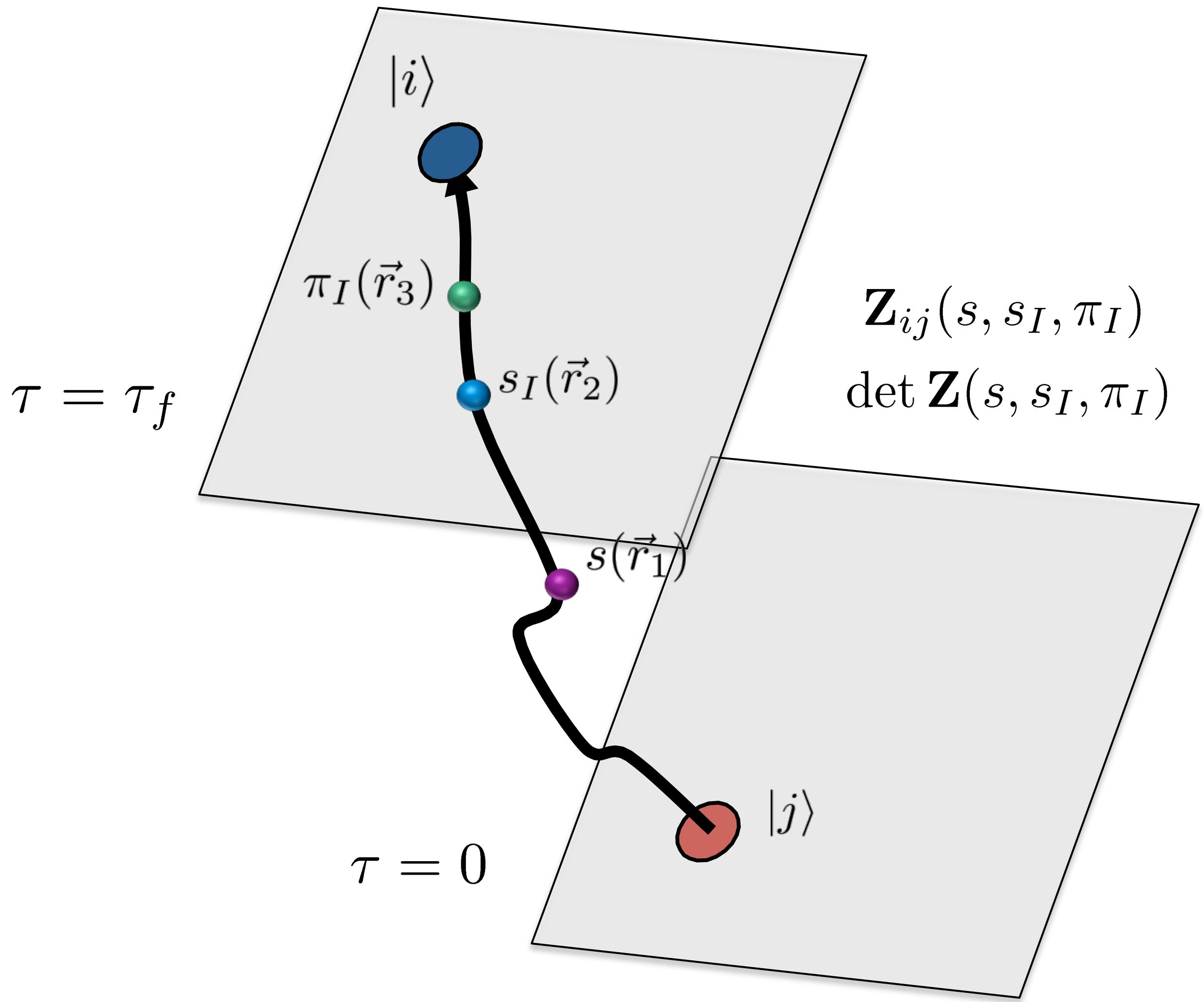
$(N^{\dagger}N)^{2}$

$$=:\sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty}ds\,\exp\left[-\frac{1}{2}s^{2}+\sqrt{-C\Delta t}\,s(N^{\dagger}N)\right]:$$



$sN^{\dagger}N$

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.


$|i\rangle$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$\tau = \tau_f$
$s(\vec{r}_1)$
$\mathbf{Z}_{ij}(s, s_I, \pi_I)$
$\det \mathbf{Z}(s, s_I, \pi_I)$
$|j\rangle$
$\tau = 0$

We first consider the leading order chiral EFT interaction on the lattice in the Grassmann path integral formalism

$$\mathcal{Z} = \int DcDc^* \exp\left[-S\left(c^*, c\right)\right]$$

$$S(c^*, c) = S_{\text{free}}(c^*, c) + S_{\text{int}}(c^*, c)$$

$$S_{\text{free}}(c^*, c) = \sum_{\vec{n},n_t,i} \boxed{c_i^*(\vec{n}, n_t)\left[c_i(\vec{n}, n_t+1) - c_i(\vec{n}, n_t)\right]} \rightarrow c_i^* \frac{\partial c_i}{\partial t}$$

$$-\frac{\alpha_t}{2m} \sum_{\vec{n},n_t,i} \sum_{l=1,2,3} \boxed{c_i^*(\vec{n}, n_t)\left[c_i(\vec{n}+\hat{l}, n_t) - 2c_i(\vec{n}, n_t) + c_i(\vec{n}-\hat{l}, n_t)\right]}$$

$$\rightarrow c_i^* \frac{\partial^2 c_i}{\partial x_l^2}$$

It is convenient to view c without indices as a column vector and c^* without indices as a row vector

$$c^* = \left[c^*_{\uparrow,p} c^*_{\downarrow,p} c^*_{\uparrow,n} c^*_{\downarrow,n}\right] \qquad c = \begin{bmatrix} c_{\uparrow,p} \\ c_{\downarrow,p} \\ c_{\uparrow,n} \\ c_{\downarrow,n} \end{bmatrix}$$

The first interaction we consider is the short-range interaction between nucleons which is independent of spin and isospin

$$S^{C}_{\text{int}}(c^*, c) = \alpha_t \tfrac{C}{2} \textstyle\sum_{\vec{n}, n_t} \left[c^*(\vec{n}, n_t) c(\vec{n}, n_t)\right]^2$$

Using the auxiliary field s, we can write this interaction as

$$\exp\left[-S^{C}_{\text{int}}(c^*, c)\right] = \textstyle\int Ds \ \exp\left[-S_{ss}(s) - S_s(c^*, c, s)\right]$$

where

$$S_{ss}(s) = \tfrac{1}{2} \textstyle\sum_{\vec{n}, n_t} s^2(\vec{n}, n_t)$$

$$S_s(c^*, c, s) = \sqrt{-C\alpha_t} \textstyle\sum_{\vec{n}, n_t} s(\vec{n}, n_t) c^*(\vec{n}, n_t) c(\vec{n}, n_t)$$

Next we have the short-range interaction dependent on isospin

$$S_{\text{int}}^{C'}(c^*, c) = \alpha_t \frac{C'}{2} \sum_{\vec{n}, n_t, I} \left[c^*(\vec{n}, n_t) \tau_I c(\vec{n}, n_t) \right]^2$$

where we are using the Pauli matrices in isospin space

$$\tau_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_{\text{isospin}} \qquad \tau_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}_{\text{isospin}} \qquad \tau_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}_{\text{isospin}}$$

In terms of three auxiliary fields s_I, we can write the interaction as

$$\exp\left[-S_{\text{int}}^{C'}(c^*, c) \right] = \int \prod_I Ds_I \exp\left[-S_{s_I s_I}(s_I) - S_{s_I}(c^*, c, s_I) \right]$$

$$S_{s_I s_I}(s_I) = \frac{1}{2} \sum_{\vec{n}, n_t, I} s_I^2(\vec{n}, n_t)$$

$$S_{s_I}(c^*, c, s_I) = \sqrt{-C' \alpha_t} \sum_{\vec{n}, n_t, I} s_I(\vec{n}, n_t) c^*(\vec{n}, n_t) \tau_I c(\vec{n}, n_t)$$

The remaining interaction is the one pion exchange potential (OPEP). We will not include time derivatives in the free pion action, and hence the the pion is not treated as a dynamical field. Instead it resembles an auxiliary field that produces an exchange potential for the nucleons.

$$\exp\left[-S_{\mathrm{int}}^{\mathrm{OPEP}}(c^*,c)\right] = \int \prod_I D\pi_I \exp\left[-S_{\pi_I\pi_I}(\pi_I) - S_{\pi_I}(c^*,c,\pi_I)\right]$$

$$S_{\pi_I\pi_I}(\pi_I) = \tfrac{1}{2}\alpha_t m_\pi^2 \sum_{\vec{n},n_t,I} \pi_I^2(\vec{n},n_t)$$
$$-\tfrac{1}{2}\alpha_t \sum_{\vec{n},n_t,I,\hat{l}} \pi_I(\vec{n},n_t)\left[\pi_I(\vec{n}+\hat{l},n_t) - 2\pi_I(\vec{n},n_t) + \pi_I(\vec{n}-\hat{l},n_t)\right]$$

The pion coupling to the nucleon is

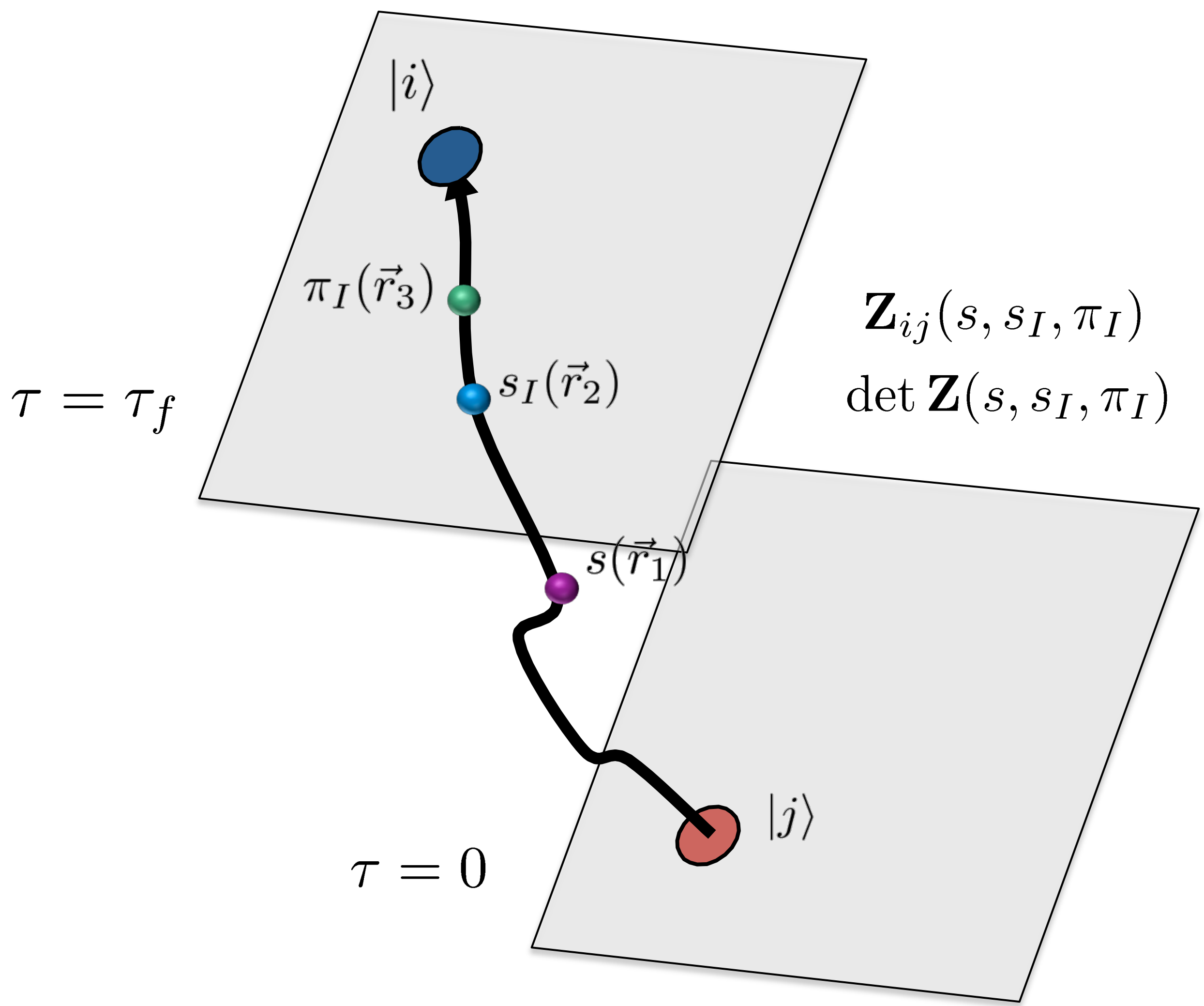
$$S_{\pi_I}(c^*, c, \pi_I) = \tfrac{g_A \alpha_t}{2 f_\pi} \textstyle\sum_{\vec{n}, n_t, k, I} \Delta_k \pi_I(\vec{n}, n_t) c^*(\vec{n}, n_t) \sigma_k \tau_I c(\vec{n}, n_t)$$

where g_A is the axial charge, f_π is the pion decay constant, and we have used the Pauli spin matrices

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_{\text{spin}} \qquad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}_{\text{spin}} \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}_{\text{spin}}$$

And the gradient of the pion field is

$$\Delta_l \pi_I(\vec{n}, n_t) = \tfrac{1}{2} \left[\pi_I(\vec{n} + \hat{l}, n_t) - \pi_I(\vec{n} - \hat{l}, n_t) \right]$$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$|j\rangle$
$\tau = 0$

We can re-express everything in terms of normal-ordered transfer matrix operators

$$\mathcal{Z} = \int Ds \prod_I \left(Ds_I D\pi_I\right)$$
$$\exp\left[-S_{ss}(s) - S_{s_I s_I}(s_I) - S_{\pi_I \pi_I}(\pi_I)\right] \mathrm{Tr}\left\{M^{(L_t-1)} \cdots M^{(0)}\right\}$$

where

$$M^{(n_t)} = : \exp\left[-H^{(n_t)}(a^\dagger, a, s, s_I, \pi_I)\alpha_t\right] :$$

$$H^{(n_t)}(a^\dagger, a, s, s_I, \pi_I)\alpha_t = H_{\text{free}}\alpha_t + S_s^{(n_t)}(a^\dagger, a, s) + S_{s_I}^{(n_t)}(a^\dagger, a, s_I) + S_{\pi_I}^{(n_t)}(a^\dagger, a, \pi_I)$$

with

$$S_s^{(n_t)}(a^\dagger, a, s) = \sqrt{-C\alpha_t} \sum_{\vec{n}} s(\vec{n}, n_t) a^\dagger(\vec{n}) a(\vec{n})$$

$$S_{s_I}^{(n_t)}(a^\dagger, a, s_I) = \sqrt{-C'\alpha_t} \sum_{\vec{n}, I} s_I(\vec{n}, n_t) a^\dagger(\vec{n}) \tau_I a(\vec{n})$$

$$S_{\pi_I}^{(n_t)}(a^\dagger, a, \pi_I) = \frac{g_A \alpha_t}{2 f_\pi} \sum_{\vec{n}, k, I} \Delta_k \pi_I(\vec{n}, n_t) a^\dagger(\vec{n}) \sigma_k \tau_I a(\vec{n})$$

For the auxiliary-field Monte Carlo calculation we compute

$$Z(L_t) = \int Ds \prod_I (Ds_I D\pi_I)$$
$$= \exp[-S_{ss}(s) - S_{s_I s_I}(s_I) - S_{\pi_I \pi_I}(\pi_I)] Z(s, s_I, \pi_I, L_t)$$

where

$$Z(s, s_I, \pi_I, L_t) = \det \mathbf{Z}(s, s_I, \pi_I, L_t)$$

and the matrix of single nucleon amplitudes is

$$\mathbf{Z}_{ij}(s, s_I, \pi_I, L_t) = \langle f_i | M^{(L_t-1)} \cdots M^{(0)} | f_j \rangle$$

We store the set of vectors for each single-particle initial state at each time step

$$|v_j^{(n_t)}\rangle = M^{(n_t-1)} \cdots M^{(0)}|f_j\rangle$$

as well as the dual vectors at each time step propagating in the reverse temporal direction

$$\langle v_i^{(n_t)}| = \langle f_i|M^{(L_t-1)} \cdots M^{(n_t)}$$

These are useful in computing the update to an auxiliary field value at time step n_t, using the following relations:

$$Z(s, s_I, \pi_I, L_t) = \det \mathbf{Z}(s, s_I, \pi_I, L_t)$$

$$\mathbf{Z}_{ij}(s, s_I, \pi_I, L_t) = \langle v_i^{(n_t+1)}|M^{(n_t)}(s, s_I, \pi_I)|v_j^{(n_t)}\rangle$$

Hybrid Monte Carlo

We want to do efficient nonlocal updates of the auxiliary and pion fields. Suppose we want to sample configurations according to the target probability

$$P_{\text{target}}(s) \propto \exp[-V(s)]$$

Hybrid Monte Carlo does this by introducing a conjugate momentum variable p_s for each variable s and sampling according classical molecular dynamics to the target probability

$$P_{\text{target}}[s, p_s] \propto \exp\{-H(s, p_s)\}$$

$$H(s, p_s) \equiv \frac{1}{2}\sum_{\vec{n},n_t}[p_s(\vec{n}, n_t)]^2 + V(s)$$

Gottlieb, Liu, Toussaint, Renken, Sugar, Phys. Rev. D35, 2531 (1987)

Duane, Kennedy, Pendleton, Roweth, Phys. Lett. B195, 216 (1987)

We start by selecting the initial p_s configuration according to the random Gaussian distribution

$$P[p_s^0(\vec{n}, n_t)] \propto \exp\left\{-\tfrac{1}{2}\left[p_s^0(\vec{n}, n_t)\right]^2\right\}$$

Then we do classical molecular dynamics updates of p_s and s which keep $H(s,\, p_s)$ approximately fixed. We use the leapfrog method which gives p_s a half step at the beginning and half step at the end, with full steps in between. In contrast, s gets full steps at every stage.

Initial half step for p_s:

$$\tilde{p}_s^0(\vec{n}, n_t) = p_s^0(\vec{n}, n_t) - \tfrac{\varepsilon_{\text{step}}}{2}\left[\tfrac{\partial V(s)}{\partial s(\vec{n}, n_t)}\right]_{s=s^0}$$

Full steps for s and p_s:

$$s^{i+1}(\vec{n}, n_t) = s^i(\vec{n}, n_t) + \varepsilon_{\text{step}} \tilde{p}_s^i(\vec{n}, n_t)$$

$$\tilde{p}_s^{i+1}(\vec{n}, n_t) = \tilde{p}_s^i(\vec{n}, n_t) - \varepsilon_{\text{step}} \left[\frac{\partial V(s)}{\partial s(\vec{n}, n_t)}\right]_{s=s^{i+1}}$$

Cut the last step for p_s so it is a half step:

$$p_s^{N_{\text{step}}}(\vec{n}, n_t) = \tilde{p}_s^{N_{\text{step}}}(\vec{n}, n_t) + \frac{\varepsilon_{\text{step}}}{2} \left[\frac{\partial V(s)}{\partial s(\vec{n}, n_t)}\right]_{s=s^0}$$

We accept the new configurations for s and p_s if the uniform random number r between 0 and 1 satisfies

$$r < \exp\left[-H(s^{N_{\text{step}}}, p_s^{N_{\text{step}}}) + H(s^0, p_s^0)\right]$$

Then return back and repeat the steps listed above.