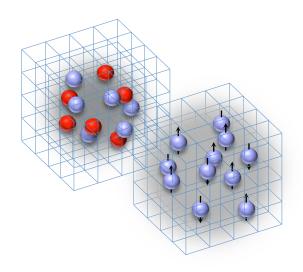
# Lattice Methods for Nuclear Physics

Lecture 1: Basic Theory and Formalism

Dean Lee (NC State)
Nuclear Lattice EFT Collaboration

TALENT School on Nuclear Quantum Monte Carlo Methods North Carolina State University July 20, 2016

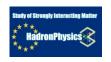
















# Lectures

Lecture 1: Basic Theory and Formalism

Lecture 2: Worldlines and Quantum Fields

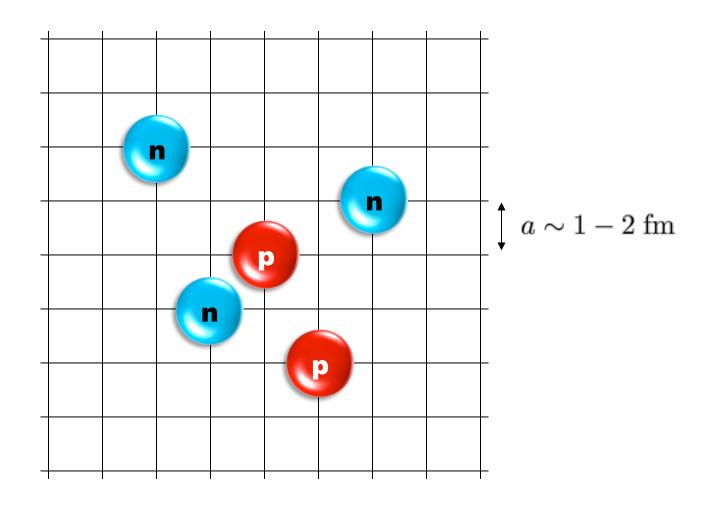
Lecture 3: Auxiliary Fields and Projection Monte Carlo

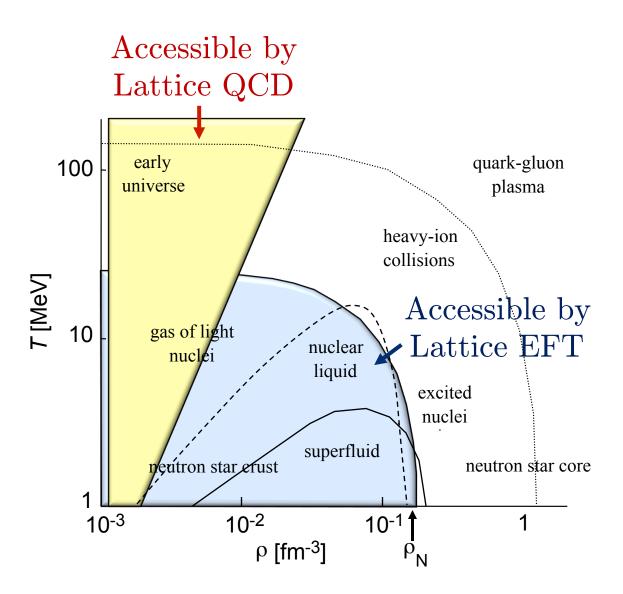
Lecture 4: Chiral Effective Field Theory on the Lattice I

Lecture 5: Chiral Effective Field Theory on the Lattice II

Lecture 6: Adiabatic Projection Method

# Lattice effective field theory





### Early lattice EFT papers on nuclear physics

Brockman, Frank, PRL 68 (1992) 1830

Shushpanov, Smilga, Phys. Rev. D59 (1999) 054013

Müller, Koonin, Seki, van Kolck, PRC 61 (2000) 044320

Lewis, Ouimet, PRD 64 (2001) 034005

Chandrasekharan, Pepe, Steffen, Wiese, JHEP 12 (2003) 35

D.L., Borasoy, Schaefer, PRC 70 (2004) 014007

### Early lattice EFT papers on cold atoms

Chen, Kaplan, PRL 92 (2004) 257002

Wingate, cond-mat/0502372

D.L., Schaefer, PRC 73 (2006) 015202

Bulgac, Drut, Magierski, PRL 96 (2006) 090404

Burovski, Prokofev, Svistunov, PRL 96 (2006) 160402

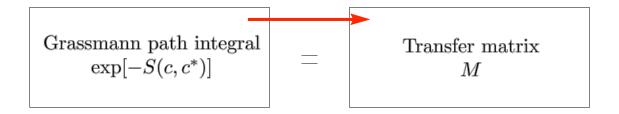
#### Review articles

D. L., Prog. Part. Nucl. Phys. 92 (2009) 117

Drut, Nicholson, J. Phys. G: Nucl. Part. Phys. 40 (2013) 043101

# Exact equivalence of lattice formulations

We show the exact equivalence between the lattice path integrals and transfer matrix operators.



We discuss the case of fermionic particles, however the case for bosonic particles is also handled by giving the fermions fictitious labels to make them distinguishable and then symmetrizing over the fictitious labels.

For simplicity we discuss the example of two-component fermions on the lattice with contact interactions

D.L., Prog. Part. Nucl. Phys. 63 (2009) 117

### Grassmann path integral

The path integral formulation is perhaps the most general framework for quantum fields. This is the formalism which extends rigorously to gauge fields. Convenient for the simple derivation of exact conservation laws, Noether currents, and Feynman diagram rules.

Let us consider anticommuting Grassmann fields for two-component fermions on a spacetime lattice

$$c_{\uparrow}(\vec{n}, n_t), c_{\downarrow}(\vec{n}, n_t), c_{\uparrow}^*(\vec{n}, n_t), c_{\downarrow}^*(\vec{n}, n_t)$$

The Grassmann fields are periodic in the spatial directions

$$c_i(\vec{n} + L\hat{1}, n_t) = c_i(\vec{n} + L\hat{2}, n_t) = c_i(\vec{n} + L\hat{3}, n_t) = c_i(\vec{n}, n_t)$$
$$c_i^*(\vec{n} + L\hat{1}, n_t) = c_i^*(\vec{n} + L\hat{2}, n_t) = c_i^*(\vec{n} + L\hat{3}, n_t) = c_i^*(\vec{n}, n_t)$$

and antiperiodic in the temporal direction

$$c_i(\vec{n}, n_t + L_t) = -c_i(\vec{n}, n_t)$$
  
$$c_i^*(\vec{n}, n_t + L_t) = -c_i^*(\vec{n}, n_t)$$

Why antiperiodic? Answer to this question will be an exercise. We use the standard definition for the Grassmann integration

$$\int dc_i(\vec{n}, n_t) = \int dc_i^*(\vec{n}, n_t) = 0,$$

$$\int dc_i(\vec{n}, n_t)c_i(\vec{n}, n_t) = \int dc_i^*(\vec{n}, n_t)c_i^*(\vec{n}, n_t) = 1$$
(no sum on *i*)

We note the equivalence of integration and differentiation with respect to a Grassmann variable

$$\int dc_i(\vec{n}, n_t) = \frac{\partial}{\partial c_i(\vec{n}, n_t)} \qquad \int dc_i^*(\vec{n}, n_t) = \frac{\partial}{\partial c_i^*(\vec{n}, n_t)}$$

We use the following shorthand notation for the full integration measure over all Grassmann variables

$$DcDc^* = \prod_{\vec{n}, n_t, i} dc_i(\vec{n}, n_t) dc_i^*(\vec{n}, n_t)$$

Define the local Grassmann spin densities

$$\rho_{\uparrow}^{c,c^*}(\vec{n},n_t) = c_{\uparrow}^*(\vec{n},n_t)c_{\uparrow}(\vec{n},n_t),$$
  
$$\rho_{\downarrow}^{c,c^*}(\vec{n},n_t) = c_{\downarrow}^*(\vec{n},n_t)c_{\downarrow}(\vec{n},n_t),$$

and the total Grassmann density

$$\rho^{c,c^*}(\vec{n},n_t) = \rho_{\uparrow}^{c,c^*}(\vec{n},n_t) + \rho_{\downarrow}^{c,c^*}(\vec{n},n_t)$$

Define the lattice kinetic energy "hopping" coefficients

$$w_0, w_1, w_2, w_3, \cdots$$

These are defined to give a quadratic kinetic energy as function of momentum

$$w_0 - w_1 \cos q_l + w_2 \cos 2q_l - w_3 \cos 3q_l + \dots = \frac{q_l^2}{2} \left[ 1 + O(q_l^{2\nu+2}) \right]$$

We can take different order of lattice improvement for the kinetic energy

$$O(a^0): \omega_0 = 1, \quad \omega_1 = 1, \quad \omega_2 = 0, \quad \omega_3 = 0$$
 $O(a^2): \omega_0 = \frac{5}{4}, \quad \omega_1 = \frac{4}{3}, \quad \omega_2 = \frac{1}{12}, \quad \omega_3 = 0$ 
 $O(a^4): \omega_0 = \frac{49}{36}, \quad \omega_1 = \frac{3}{2}, \quad \omega_2 = \frac{3}{20}, \quad \omega_3 = \frac{1}{90}$ 

In our simulations of nucleons, we typically use fourth-order improvement for the kinetic energy, but for illustrative simplicity we continue the discussion with the simplest case,

$$O(a^0): \omega_0 = 1, \quad \omega_1 = 1, \quad \omega_2 = 0, \quad \omega_3 = 0$$

We use lattice units where everything is divided or multiplied by powers of the spatial lattice spacing to make it dimensionless. We also define the ratio of temporal to spatial lattice spacings

$$\alpha_t = a_t/a$$

The free nonrelativistic particle lattice action in its simplest form is

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

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

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

With a contact interaction between the two components, the lattice action is

$$S(c, c^*) = S_{\text{free}}(c, c^*) + C\alpha_t \sum_{\vec{n}, n_t} \rho_{\uparrow}^{c, c^*}(\vec{n}, n_t) \rho_{\downarrow}^{c, c^*}(\vec{n}, n_t).$$

We are interested in the path integral of the exponential of the action

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

# Second quantization and the transfer matrix

Consider now fermion annihilation and creation operators. For the moment we consider just one operator each

$$\{a, a\} = \{a^{\dagger}, a^{\dagger}\} = 0$$
$$\{a, a^{\dagger}\} = 1$$

For any function of the annihilation and creation operators

$$f\left(a^{\dagger},a\right)$$

we note that the quantum-mechanical trace of the normal-ordered product satisfies the following identity relating it to a Grassmann integral

$$Tr\left[:f\left(a^{\dagger},a\right):\right] = \int dc dc^* e^{2c^*c} f(c^*,c)$$

Creutz, Found. Phys. 30 (2000) 487

The pedestrian proof consists of testing all four linearly independent functions of the annihilation and creation operators

$$f(a^{\dagger},a) = \{1,a,a^{\dagger},a^{\dagger}a\}$$
 
$$Tr\left[:f\left(a^{\dagger},a\right):\right] = \int dc dc^{*}e^{2c^{*}c}f(c^{*},c)$$

$$Tr \left[ : f\left(a^{\dagger}, a\right) : \right] \qquad \int dc dc^{*} e^{2c^{*}c} f(c^{*}, c)$$

$$= \int dc dc^{*} (1 + 2c^{*}c) f(c^{*}, c)$$

$$= \left(\frac{\partial}{\partial c^{*}}\right) (1 + 2c^{*}c) f(c^{*}, c) \left(\frac{\partial}{\partial c}\right)$$

$$= \left(\frac{\partial}{\partial c^{*}}\right) (1 + 2c^{*}c) f(c^{*}, c) \left(\frac{\partial}{\partial c}\right)$$

$$= \left(\frac{\partial}{\partial c^{*}}\right) (1 + 2c^{*}c) f(c^{*}, c) \left(\frac{\partial}{\partial c}\right)$$

$$= \left(\frac{\partial}{\partial c^{*}}\right) (1 + 2c^{*}c) f(c^{*}, c) \left(\frac{\partial}{\partial c}\right)$$

$$= \left(\frac{\partial}{\partial c^{*}}\right) (1 + 2c^{*}c) f(c^{*}, c) \left(\frac{\partial}{\partial c}\right)$$

$$= \left(\frac{\partial}{\partial c^{*}}\right) (1 + 2c^{*}c) f(c^{*}, c) \left(\frac{\partial}{\partial c}\right)$$

Let us rewrite the identity in a fancy form that starts to resemble the lattice Grassmann path integral

$$Tr\left[:f\left(a^{\dagger},a\right):\right] = \int dc(0)dc^{*}(0)e^{c^{*}(0)[c(0)-c(1)]}f\left[c^{*}(0),c(0)\right]$$
$$c(1) = -c(0)$$

This identity can be generalized to any sequential product of normal-ordered functions of the annihilation and creation operators.

$$\operatorname{Tr} \left\{ : f_{L_{t}-1}(a^{\dagger}, a) : \dots : f_{0}(a^{\dagger}, a) : \right\}$$

$$= \int DcDc^{*} \exp \left\{ \sum_{n_{t}=0}^{L_{t}-1} \sum_{\vec{n}, i} c^{*}(n_{t}) \left[ c(n_{t}) - c(n_{t}+1) \right] \right\}$$

$$\times f_{L_{t}-1} \left[ c^{*}(L_{t}-1), c(L_{t}-1) \right] \cdots f_{0} \left[ c^{*}(0), c(0) \right]$$

$$c(L_{t}) = -c(0)$$

$$DcDc^{*} \equiv dc(L_{t}-1) dc^{*}(L_{t}-1) \cdots dc(0) dc^{*}(0)$$

Let us prove this result. Let the state with no fermion be written as

$$|0\rangle$$

and the state with one fermion be written as

$$|1\rangle = a^{\dagger}|0\rangle$$

Then the set of matrix elements for all possible functions are listed as follows:

$$\langle i|: f(a^{\dagger}, a): |j\rangle = f_{ij}$$

1	$\delta_{i,j}$
a	$\delta_{i,0}\delta_{j,1}$
$a^{\dagger}$	$\delta_{i,1}\delta_{j,0}$
$a^{\dagger}a$	$\delta_{i,1}\delta_{j,1}$

Notice that we get exactly the same matrix elements with the following Grassmann variable operations:

$$\frac{\overrightarrow{\left(\frac{\partial}{\partial c^*}\right)^i} e^{c^*c} f(c^*, c) \left(\frac{\partial}{\partial c}\right)^j}{\underbrace{\left(\frac{\partial}{\partial c}\right)^j}_{c=c^*=0}} = f_{ij}$$

$$\frac{1}{c} \frac{\delta_{i,j}}{\delta_{i,0}\delta_{j,1}}$$

$$\underline{c^*} \frac{\delta_{i,1}\delta_{j,0}}{c^*c} \frac{\delta_{i,1}\delta_{j,1}}{c^*}$$

Let us define

$$\tilde{f}(c^*,c) = e^{c^*c} f(c^*,c)$$

We now have the following trace formula:

$$\sum_{i=0,1} f_{ii} = \sum_{i=0,1} \left. \overrightarrow{\left(\frac{\partial}{\partial c^*}\right)^i} \widetilde{f}(c^*,c) \overleftarrow{\left(\frac{\partial}{\partial c}\right)^i} \right|_{c=c^*=0}$$

We can also connect this trace formula with a Grassmann path integral:

$$\sum_{i=0,1} f_{ii} = \sum_{i=0,1} \overrightarrow{\left(\frac{\partial}{\partial c^*}\right)^i} \tilde{f}(c^*,c) \left(\frac{\partial}{\partial c}\right)^i \Big|_{c=c^*=0}$$

$$= \int dc dc^* (1+c^*c) \tilde{f}(c^*,c)$$

$$= \int dc dc^* e^{c^*c} \tilde{f}(c^*,c)$$

We also note the following matrix product contraction formula:

$$\sum_{j=0,1} f'_{ij} f_{jk} = \sum_{j=0,1} \left( \frac{\partial}{\partial c'^*} \right)^i \tilde{f}'(c'^*,c') \left( \frac{\partial}{\partial c'} \right)^j \left( \frac{\partial}{\partial c^*} \right)^j \tilde{f}(c^*,c) \left( \frac{\partial}{\partial c} \right)^k \right|_{c=c^*=c'=c'^*=0}$$

We connect this matrix product contraction formula with a Grassmann path integral. We first note that

$$\sum_{j=0,1} \tilde{f}'(c'^*,c') \left(\frac{\partial}{\partial c'}\right)^j \left(\frac{\partial}{\partial c^*}\right)^j \tilde{f}(c^*,c) \Big|_{c^*=c'=0}$$

$$= (-1) \sum_{j=0,1} \int dc' dc^* \tilde{f}'(c'^*,c') (1-c^*c') \tilde{f}(c^*,c)$$

And therefore we get

$$\sum_{j=0,1} f'_{ij} f_{jk} = (-1) \sum_{j=0,1} \overrightarrow{\left(\frac{\partial}{\partial c'^*}\right)^i} \int dc' dc^* \widetilde{f}'(c'^*,c') (1-c^*c') \widetilde{f}(c^*,c) \overleftarrow{\left(\frac{\partial}{\partial c}\right)^k} \Big|_{c=c'^*=0}$$

$$= (-1) \sum_{j=0,1} \overrightarrow{\left(\frac{\partial}{\partial c'^*}\right)^i} \int dc' dc^* \widetilde{f}'(c'^*,c') e^{-c^*c'} \widetilde{f}(c^*,c) \overleftarrow{\left(\frac{\partial}{\partial c}\right)^k} \Big|_{c=c'^*=0}$$

Putting everything together we get the following expression for the trace of a product of several matrices:

$$\sum_{i_0,\dots,i_{L_t-1}=0,1} [f_{L_t-1}]_{i_0 i_{L_t-1}} [f_{L_t-2}]_{i_{L_t-1} i_{L_t-2}} \cdots [f_0]_{i_1 i_0} =$$

$$= \int dc(0) dc^*(L_t-1) e^{c^*(L_t-1)c(0)} \qquad \text{(trace)}$$

$$\cdot e^{c^*(L_t-1)c(L_t-1)} f_{L_t-1}(c^*(L_t-1), c(L_t-1)) \qquad \text{(matrix element)}$$

$$\cdot (-1) dc(L_t-1) dc^*(L_t-2) e^{-c^*(L_t-2)c(L_t-1)} \qquad \text{(contraction)}$$

$$\cdots$$

$$\cdot (-1) dc(1) dc^*(0) e^{-c^*(0)c(1)} \qquad \text{(contraction)}$$

$$\cdot e^{c^*(0)c(0)} f_0(c^*(0), c(0)) \qquad \text{(matrix element)}$$

We now collect the integral measure terms and can reorder as

$$dc(0)dc^*(L_t - 1)(-1)dc(L_t - 1)dc^*(L_t - 2)\cdots(-1)dc(1)dc^*(0)$$
$$= dc(L_t - 1)dc^*(L_t - 1)\cdots dc(0)dc^*(0)$$

We conclude that

$$\operatorname{Tr}\left\{: f_{L_{t}-1}(a^{\dagger}, a) : \dots : f_{0}(a^{\dagger}, a) :\right\}$$

$$= \sum_{i_{0}, \dots, i_{L_{t}-1} = 0, 1} [f_{L_{t}-1}]_{i_{0}i_{L_{t}-1}} [f_{L_{t}-2}]_{i_{L_{t}-1}i_{L_{t}-2}} \cdots [f_{0}]_{i_{1}i_{0}}$$

$$= \int DcDc^{*} \exp\left\{\sum_{n_{t}=0}^{L_{t}-1} \sum_{\vec{n}, i} c^{*}(n_{t}) \left[c(n_{t}) - c(n_{t}+1)\right]\right\}$$

$$\times f_{L_{t}-1} \left[c^{*}(L_{t}-1), c(L_{t}-1)\right] \cdots f_{0} \left[c^{*}(0), c(0)\right]$$

$$c(L_{t}) = -c(0)$$

An exactly analogous proof can be applied to the case with more fermionic degrees of freedom. For any number of fermion annihilation and creation operators residing on the spatial lattice sites, we have

$$\operatorname{Tr}\left\{: f_{L_{t}-1}\left[a_{i'}^{\dagger}(\vec{n}'), a_{i}(\vec{n})\right] : \dots : f_{0}\left[a_{i'}^{\dagger}(\vec{n}'), a_{i}(\vec{n})\right] : \right\}$$

$$= \int DcDc^{*} \exp\left\{\sum_{n_{t}=0}^{L_{t}-1} \sum_{\vec{n}, i} c_{i}^{*}(\vec{n}, n_{t}) \left[c_{i}(\vec{n}, n_{t}) - c_{i}(\vec{n}, n_{t}+1)\right]\right\}$$

$$\times f_{L_{t}-1}\left[c_{i'}^{*}(\vec{n}', L_{t}-1), c_{i}(\vec{n}, L_{t}-1)\right] \cdots f_{0}\left[c_{i'}^{*}(\vec{n}', 0), c_{i}(\vec{n}, 0)\right]$$

with antiperiodic time boundary conditions

$$c_i(\vec{n}, L_t) = -c_i(\vec{n}, 0)$$

We now define the free nonrelativistic lattice Hamiltonian in its simplest form

$$H_{\text{free}} = -\frac{1}{2m} \sum_{\vec{n},i} \sum_{l=1,2,3} a_i^{\dagger}(\vec{n}) \left[ a_i(\vec{n} + \hat{l}) - 2a_i(\vec{n}) + a_i(\vec{n} - \hat{l}) \right]$$

$$\rightarrow a_i^{\dagger} \frac{\partial^2 a_i}{\partial x_l^2}$$

We also define the following density operators

$$\rho_{\uparrow}(\vec{n}) = a_{\uparrow}^{\dagger}(\vec{n})a_{\uparrow}(\vec{n}) \qquad \rho_{\downarrow}(\vec{n}) = a_{\downarrow}^{\dagger}(\vec{n})a_{\downarrow}(\vec{n})$$
$$\rho(\vec{n}) = \rho_{\uparrow}(\vec{n}) + \rho_{\downarrow}(\vec{n})$$

So now the same Grassmann path integral we had defined before

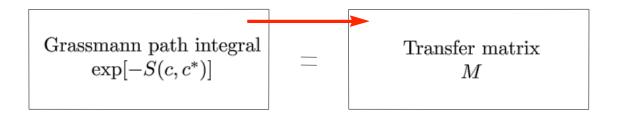
$$\mathcal{Z} = \int DcDc^* \exp\left[-S(c, c^*)\right]$$

can be rewritten in terms of the quantum-mechanical trace of the product of normal-ordered transfer matrices

$$\mathcal{Z} = Tr\left(M^{L_t}\right)$$

$$M =: \exp\left[-H_{\text{free}}\alpha_t - C\alpha_t \sum_{\vec{n}} \rho_{\uparrow}(\vec{n})\rho_{\downarrow}(\vec{n})\right]:$$

This demonstrates the exact equivalence of the two lattice formulations for any spatial and temporal lattice spacings.



#### Markov chains

We will be discussing several types of Markov chain algorithms. It is useful to review the elements and theory of Markov chains. Consider a chain of configurations labeled by order of selection. We call this integer-valued label the computation step.

Let us denote the probability of selecting configuration A at computation step n as

Suppose we have selected configuration A at computation step n. The probability that we select configuration B at computation step n+1 is denoted

$$W(A \to B)$$

This transition probability is chosen to be independent of n and independent of the history of configurations selected prior to selecting A at computation step n. This defines a Markov chain.

We note that

$$\begin{split} P(A,n+1) &= P(A,n) + \sum_{B \neq A} W(B \rightarrow A) P(B,n) \\ &- \sum_{B \neq A} W(A \rightarrow B) P(A,n) \end{split}$$

We now define the notion of ergodicity. Suppose we are at configuration A at computation step, n. Let  $S_A$  be the set of all positive integers m, such that the return probability to A is nonzero

$$S_A = \{ m | P(A, n+m) > 0 \}$$

If the set  $S_A$  is not empty, then we say that A is positive recurrent. If the greatest common divisor of the set of integers in  $S_A$  is 1, then we say that A is aperiodic. If all of the configurations connected by the Markov chain are recurrent and aperiodic, then the Markov chain is said to be ergodic. If the Markov chain is ergodic and all configurations are connected by the graph of nonzero transitions in the Markov chain, then there is a unique equilibrium distribution that is reached in the limit of large number of computation steps that is independent of the initial conditions.

$$\lim_{\tau \to \infty} P(C, \tau) \to p(C)$$

Serfozo, "Basics of Applied Stochastic Processes", (Berlin: Springer-Verlag) 2009

#### Detailed balance

We want the equilibrium probability distribution to be

$$p_{\text{target}}(C)$$

One way to do this is to require

$$W(A \to B)p_{\text{target}}(A) = W(B \to A)p_{\text{target}}(B)$$

for every pair of configurations A and B. This condition is called detailed balance.

If the Markov chain is ergodic and all configurations are connected, then after many computation steps we reach the unique equilibrium distribution, which satisfies the stationary condition

$$\sum_{B \neq A} W(A \to B) p(A) = \sum_{B \neq A} W(B \to A) p(B)$$

Comparing with the detailed balance condition, we conclude that

$$p(A) = p_{\text{target}}(A)$$

for all configurations A.

# Metropolis algorithm

One popular method for generating the desired detailed balance condition is the Metropolis algorithm

Metropolis, Teller, Rosenbluth, J. Chem. Phys. 21 (1953) 1087

$$W(A \to B) = \begin{cases} \frac{p_{\text{target}}(B)}{p_{\text{target}}(A)} & p_{\text{target}}(B) \le p_{\text{target}}(A) \\ 1 & p_{\text{target}}(B) > p_{\text{target}}(A) \end{cases}$$

Usually the transition probability can be divided in terms of a proposed move probability and an acceptance probability,

$$W(A \to B) = W_{\text{propose}}(A \to B)W_{\text{accept}}(A \to B)$$

And quite often the proposed move probability is symmetric

$$W_{\text{propose}}(A \to B) = W_{\text{propose}}(B \to A)$$

However this does not need to be the case. One can design useful algorithms where there is some guiding involved in the proposed moves. It is also not necessary that you use only one type of update. If you maintain detailed balance for each type of update process, then you also recover the target probability distribution.

Once your Markov chain is set up properly, you can now compute observables such as

$$\langle O \rangle = \frac{\sum_{A} O(A) p_{\text{target}}(A)}{\sum_{A} p_{\text{target}}(A)}$$

by computing the average

$$\langle O \rangle = \frac{\sum_{n=1,N} O(A_n)}{N}$$

for large N from your Markov chain. However you can also do some reweighting and sample the Markov chain according to some other probability distribution  $q_{\text{target}}(A)$ . This may be necessary if  $p_{\text{target}}(A)$  is not positive semi-definite and so cannot be treated as a probability distribution. In that case you can for example take

$$q_{\text{target}}(A) = |p_{\text{target}}(A)|$$

With the reweighted Markov chain, you then compute averages using

$$\langle O \rangle = \frac{\sum_{n=1,N} O(A_n) p_{\text{target}}(A_n) / q_{\text{target}}(A_n)}{\sum_{n=1,N} p_{\text{target}}(A_n) / q_{\text{target}}(A_n)}$$

#### Exercise 1

Let

$$M = \begin{bmatrix} 1.1 & 0.1 & 0.1 \\ 0.1 & 0.8 & 0.1 \\ 0.1 & 0.1 & 0.8 \end{bmatrix} \qquad f(n) = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} M^n \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

Construct a Markov process using the Metropolis algorithm to compute:

by sampling over all terms in the matrix product

$$\left[\begin{array}{ccc} 1 & 0 & 0\end{array}\right] M \cdot M \cdot \cdots \cdot M \left[\begin{array}{c} 1 \\ 0 \\ 0\end{array}\right]$$

Determine the exact result and compare with your Monte Carlo simulation results and verify agreement to at least five digit accuracy.

#### Exercise 2

Show what equivalent expression we get in the transfer matrix operator formalism if we take periodic boundary conditions in time:

$$c(L_t) = +c(0)$$

$$\int DcDc^* \exp\left\{\sum_{n_t=0}^{L_t-1} \sum_{\vec{n},i} c^*(n_t) \left[c(n_t) - c(n_t+1)\right]\right\} \times f_{L_t-1} \left[c^*(L_t-1), c(L_t-1)\right] \cdots f_0 \left[c^*(0), c(0)\right] = ?$$