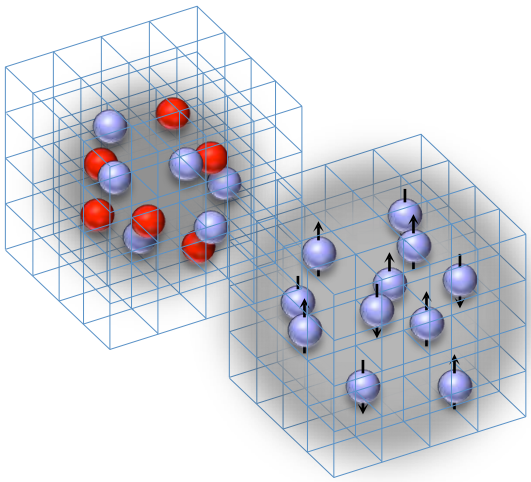
Nuclear Lattice Simulations

Lecture 1: Lattice Field Theory and Monte Carlo Methods

Dean Lee
Facility for Rare Isotope Beams
Michigan State University
Nuclear Lattice EFT Collaboration



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Lectures

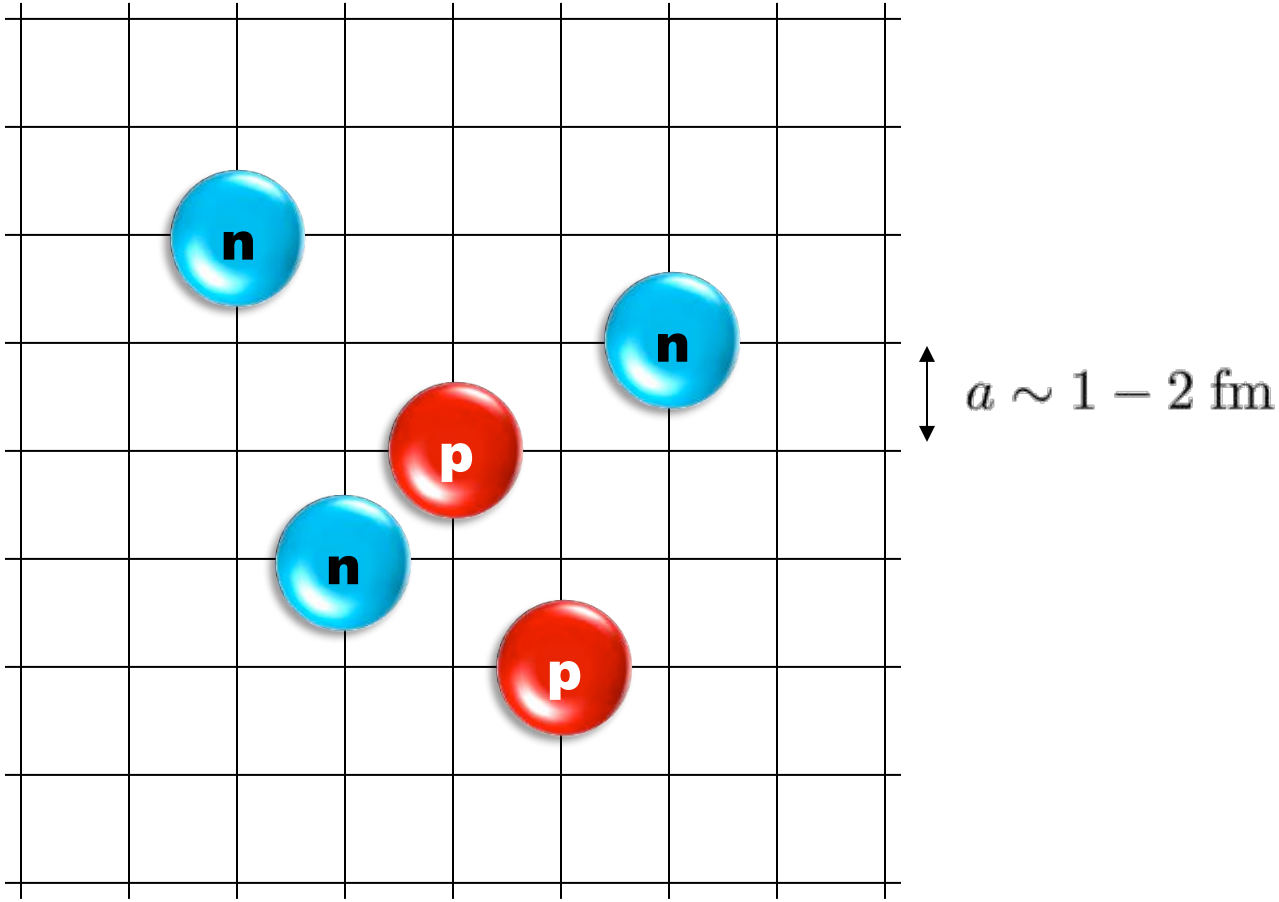
Lecture 1: Lattice Field Theory and Monte Carlo Methods

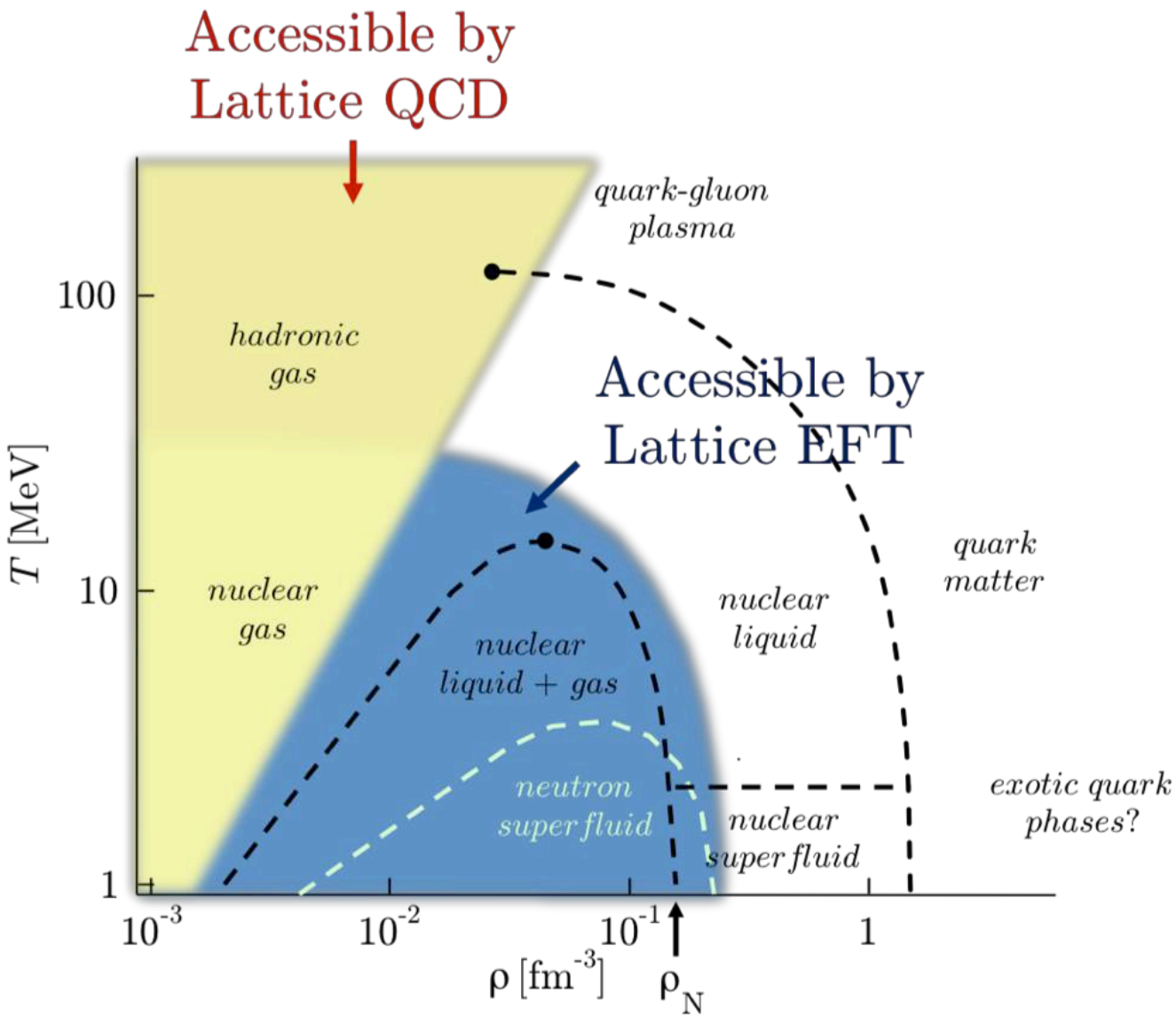
Lecture 2: Path Integrals, Transfer Matrices, and Auxiliary Fields

Lecture 3: Chiral Effective Field Theory on the Lattice

Lecture 4: Applications of Nuclear Lattice Simulations

Lattice effective field theory

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phases?
T [MeV]
100
10
1
10^-3
10^-2
10^-1
1
ρ [fm^-3]
ρ_N

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

Markov chain Monte Carlo

We will be discussing several different Monte Carlo 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

$$P(A, n)$$

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

$$P(A, n+1) = P(A, n) + \sum_{B \neq A} W(B \to A) P(B, n) - \sum_{B \neq A} W(A \to B) P(A, n)$$

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

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

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

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

Free scalar quantum field on the lattice

We consider a relativistic free scalar quantum field in 3 + 1 dimensions, three spatial dimensions plus time. We work in Euclidean space where time t is replaced by Euclidean or imaginary time x_4.

$$x = (\vec{x}, x_4)$$

The Euclidean action for the free scalar field is

$$S_E[\phi] = \frac{1}{2} \int d^4x \phi(x)(-\Box + M^2)\phi(x)$$

where

$$\Box = \sum_\mu \partial_\mu \partial_\mu$$

Rothe, Lattice Gauge Theories, Second Edition,
World Scientific Lecture Notes in Physics, Vol. 59, 1997

We can calculate any expectation value of products of quantum fields by computing the ratio of path (or functional) integrals

$$\langle \phi(x)\phi(y)\cdots\rangle = \frac{\int D\phi\phi(x)\phi(y)\cdots e^{-S_E[\phi]}}{\int D\phi e^{-S_E[\phi]}}$$

where the path integral measure is

$$D\phi = \prod_x d\phi(x)$$

We now put this system on a lattice with periodic boundary conditions

$$L \times L \times L \times L_t \ \text{ lattice}$$

$$x_\mu \to n_\mu a$$

$$\phi(x) \to \phi(na)$$

$$\phi(na + \hat{1}La) = \phi(na)$$

$$\phi(na + \hat{2}La) = \phi(na)$$

$$\phi(na + \hat{3}La) = \phi(na)$$

$$\phi(na + \hat{4}L_t a) = \phi(na)$$

The Euclidean time duration, $L_t a$, will be the inverse temperature β. On the lattice we also make the replacements

$$\int d^4x \to a^4 \sum_n$$

$$D\phi(x) \to \prod_n d\phi(na)$$

$$\Box\phi(x) \to \frac{1}{a^2}\hat{\Box}\phi(na)$$

where

$$\hat{\Box}\phi(na) = \sum_\mu (\phi(na + \hat{\mu}a) - 2\phi(na) + \phi(na - \hat{\mu}a))$$

To simplify the notation further we redefine the fields and mass parameter multiplied by the lattice spacing to render it dimensionless.

$$\hat{\phi}_n = a\phi(na)$$
$$\hat{M} = aM$$

Then the expectation value of products of quantum fields can be written as

$$\langle \hat{\phi}_n \hat{\phi}_m \cdots \rangle = \frac{\int \prod_l d\hat{\phi}_l \hat{\phi}_n \hat{\phi}_m \cdots e^{-S_E[\hat{\phi}]}}{\int \prod_l d\hat{\phi}_l e^{-S_E[\hat{\phi}]}}$$

where

$$S_E = -\sum_{n,\mu} \hat{\phi}_n \hat{\phi}_{n+\hat{\mu}} + \frac{1}{2}(8 + \hat{M}^2) \sum_n \hat{\phi}_n \hat{\phi}_n$$

We can also write

$$S_E = \frac{1}{2} \sum_{n,m} \hat{\phi}_n K_{n,m} \hat{\phi}_m$$

where

$$K_{n,m} = -\sum_{\mu}[\delta_{n+\hat{\mu},m} + \delta_{n-\hat{\mu},m} - 2\delta_{n,m}] + \hat{M}^2\delta_{n,m}$$

Using this notation, the two-field expectation value called the Euclidean propagator is given by

$$\langle\hat{\phi}_n\hat{\phi}_m\rangle = \frac{\int\prod_l d\hat{\phi}_l\hat{\phi}_n\hat{\phi}_m e^{-\frac{1}{2}\sum_{n,m}\hat{\phi}_n K_{n,m}\hat{\phi}_m}}{\int\prod_l d\hat{\phi}_l e^{-\frac{1}{2}\sum_{n,m}\hat{\phi}_n K_{n,m}\hat{\phi}_m}}$$

$K_{n,m}$ is a symmetric positive-definite matrix which only depends on the vector difference $n - m$. We can compute the square root and define

$$\hat{\phi}'_n = \sum_m K^{\frac{1}{2}}_{n,m}\hat{\phi}_m$$

We can also invert to get

$$\hat{\phi}_n = \sum_m K^{-\frac{1}{2}}_{n,m} \hat{\phi}'_m$$

We now do a change of variables in the path integration and get

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = \frac{\int \prod_l d\hat{\phi}_l \hat{\phi}_n \hat{\phi}_m e^{-\frac{1}{2}\sum_{n,m} \hat{\phi}_n K_{n,m} \hat{\phi}_m}}{\int \prod_l d\hat{\phi}_l e^{-\frac{1}{2}\sum_{n,m} \hat{\phi}_n K_{n,m} \hat{\phi}_m}}$$

$$= \frac{\int \prod_l d\hat{\phi}'_l \sum_{n'} K^{-\frac{1}{2}}_{n,n'} \hat{\phi}'_{n'} \sum_{m'} K^{-\frac{1}{2}}_{m,m'} \hat{\phi}'_{m'} e^{-\frac{1}{2}\sum_j \hat{\phi}'_j \hat{\phi}'_j}}{\int \prod_l d\hat{\phi}'_l e^{-\frac{1}{2}\sum_j \hat{\phi}'_j \hat{\phi}'_j}}$$

It is straightforward to calculate the second moments of this simple Gaussian distribution

$$\frac{\int \prod_l d\hat{\phi}'_l \hat{\phi}'_{n'} \hat{\phi}'_{m'} e^{-\frac{1}{2}\sum_j \hat{\phi}'_j \hat{\phi}'_j}}{\int \prod_l d\hat{\phi}'_l e^{-\frac{1}{2}\sum_j \hat{\phi}'_j \hat{\phi}'_j}} = \delta_{n',m'}$$

The Euclidean propagator is then

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = \sum_{n'} K^{-\frac{1}{2}}_{n,n'} K^{-\frac{1}{2}}_{m,n'} = \sum_{n'} K^{-\frac{1}{2}}_{n,n'} K^{-\frac{1}{2}}_{n',m} = K^{-1}_{n,m}$$

In order to compute this inverse matrix, we first compute the Fourier transform of

$$K_{n,m} = -\sum_{\mu} [\delta_{n+\hat{\mu},m} + \delta_{n-\hat{\mu},m} - 2\delta_{n,m}] + \hat{M}^2 \delta_{n,m}$$

and get the momentum-space function

$$\begin{aligned} \tilde{K}(k) = \sum_{l} K_{m+l,m} e^{-ik\cdot l} &= -\sum_{\mu} [e^{-ik\cdot\hat{\mu}} + e^{+ik\cdot\hat{\mu}} - 2] + \hat{M}^2 \\ &= 2\sum_{\mu} [1 - \cos(k_\mu)] + \hat{M}^2 \end{aligned}$$

The allowed momentum modes on the lattice in our periodic box are

$$k_1 = 0, 2\pi/L, 4\pi/L, \cdots 2(L-1)\pi/L$$
$$k_2 = 0, 2\pi/L, 4\pi/L, \cdots 2(L-1)\pi/L \quad k_4 = 0, 2\pi/L_t, 4\pi/L_t, \cdots 2(L_t-1)\pi/L_t$$
$$k_3 = 0, 2\pi/L, 4\pi/L, \cdots 2(L-1)\pi/L$$

To convert back to coordinate space, we compute the inverse Fourier transform

$$K_{n,m} = \frac{1}{L^3 L_t} \sum_k \tilde{K}(k) e^{ik\cdot(n-m)}$$

and we can construct the inverse matrix as

$$K^{-1}_{n,m} = \frac{1}{L^3 L_t} \sum_k \frac{1}{\tilde{K}(k)} e^{ik\cdot(n-m)}$$

We can check that this definition is in fact the matrix inverse

$$\sum_l K^{-1}_{n,l} K_{l,m} = \frac{1}{L^3 L_t} \sum_l \sum_k \frac{1}{\tilde{K}(k)} e^{ik\cdot(n-l)} \frac{1}{L^3 L_t} \sum_{k'} \tilde{K}(k') e^{ik'\cdot(l-m)}$$

$$= \frac{1}{L^3 L_t} \sum_k \frac{1}{\tilde{K}(k)} \tilde{K}(k) e^{ik\cdot(n-m)}$$

$$= \frac{1}{L^3 L_t} \sum_k e^{ik\cdot(n-m)} = \delta_{n,m}$$

We conclude that the Euclidean propagator is

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = K^{-1}_{n,m} = \frac{1}{L^3 L_t} \sum_k \frac{1}{2\sum_\mu [1 - \cos(k_\mu)] + \hat{M}^2} e^{ik\cdot(n-m)}$$

Exercise

Use a Markov chain Monte Carlo simulation to compute the Euclidean propagator for a real scalar field on the lattice in $3+1$ dimensions.

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = \frac{\int \prod_l d\hat{\phi}_l \hat{\phi}_n \hat{\phi}_m e^{-S_E[\hat{\phi}]}}{\int \prod_l d\hat{\phi}_l e^{-S_E[\hat{\phi}]}}$$

$$S_E = -\sum_{n,\mu} \hat{\phi}_n \hat{\phi}_{n+\hat{\mu}} + \frac{1}{2}(8 + \hat{M}^2) \sum_n \hat{\phi}_n \hat{\phi}_n$$

Take the size of the periodic box to be $L = L_t = 10$ and also set

$$\hat{M} = 1$$

Check that your simulation gives the same result as the expression

we had derived analytically

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = \frac{1}{L^3 L_t} \sum_k \frac{1}{2\sum_\mu [1 - \cos(k_\mu)] + \hat{M}^2} e^{ik\cdot(n-m)}$$

for the cases where the separation between n and m is pointing along the x-axis:

$$n - m = 0, 1\hat{1}, 2\hat{1}, \cdots (L-1)\hat{1}$$