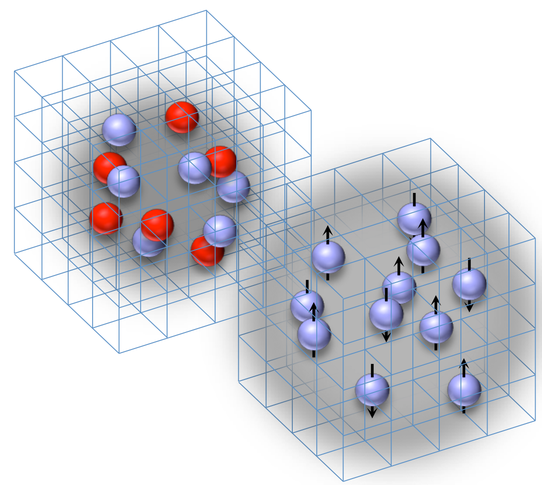
Nuclear Lattice Simulations

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

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



Swieca Summer School on Nuclear Theory
Campos do Jordão, SP, Brazil
Feburary 10-15, 2019

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

Exact equivalence of lattice formulations

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

Grassmann path integral $\exp[-S(c^*, c)]$	$=$	Transfer matrix M

We discuss the case of fermionic particles, however the case for bosonic particles is also handled by giving the fermions extra labels to make them distinguishable and then symmetrizing over the extra 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? This will become clear as we work through the correspondence between path integrals and transfer matrices. 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

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

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

$$\to c_i^* \frac{\partial c_i}{\partial t}$$

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

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

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

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

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

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

$$f(a^\dagger, a) = \{1, a, a^\dagger, a^\dagger a\}$$

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

$$\int dc dc^* e^{2c^* c} f(c^*, c)$$

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

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

$$Tr\left[: f\left(a^\dagger, a\right) :\right]$$

1	2
a	0
$a^\dagger$	0
$a^\dagger a$	1

1	2
c	0
c^*	0
$c^* c$	1

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 product of normal-ordered functions of the annihilation and creation operators. Proof is left as an exercise.

$$\begin{aligned}\mathrm{Tr}&\left\{:f_{L_t-1}(a^\dagger,a):\cdots:f_0(a^\dagger,a):\right\}\\ &=\int DcDc^*\exp\left\{\sum_{n_t=0}^{L_t-1}\sum_{\vec{n},i}c^*(n_t)\left[c(n_t)-c(n_t+1)\right]\right\}\\ &\qquad\times f_{L_t-1}\left[c^*(L_t-1),c(L_t-1)\right]\cdots f_0\left[c^*(0),c(0)\right]\end{aligned}$$

$$c(L_t) = -c(0)$$
$$DcDc^* \equiv dc(L_t-1)dc^*(L_t-1)\cdots dc(0)dc^*(0)$$

This identity can be generalized 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

$$
\begin{aligned}
&\mathrm{Tr}\left\{: f_{L_t-1}\left[a_{i'}^{\dagger}(\vec{n}'), a_i(\vec{n})\right] : \cdots : f_0\left[a_{i'}^{\dagger}(\vec{n}'), a_i(\vec{n})\right] :\right\} \\
&= \int DcDc^* \exp\left\{\sum_{n_t=0}^{L_t-1} \sum_{\vec{n},i} c_i^*(\vec{n}, n_t)\left[c_i(\vec{n}, n_t) - c_i(\vec{n}, n_t+1)\right]\right\} \\
&\quad \times f_{L_t-1}\left[c_{i'}^*(\vec{n}', L_t-1), c_i(\vec{n}, L_t-1)\right] \cdots f_0\left[c_{i'}^*(\vec{n}', 0), c_i(\vec{n}, 0)\right]
\end{aligned}
$$

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

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

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

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

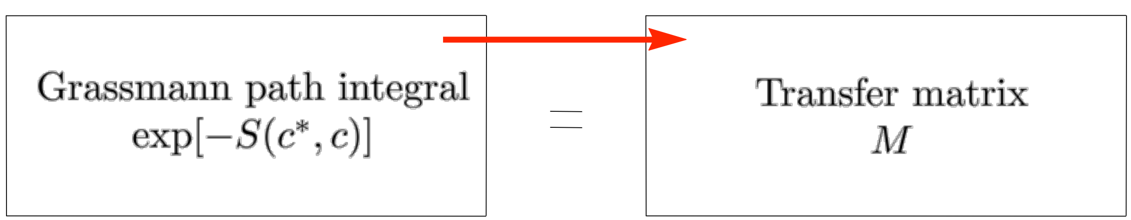
$$\mathcal{Z} = \int DcDc^* \exp\left[-S(c^*, c)\right]$$

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.



Auxiliary fields

We proved the exact equivalence between the Grassmann path integral and transfer matrix operator formalisms.

Grassmann path integral $\exp[-S(c^*,c)]$	$=$	Transfer matrix M

For our example of two-component fermions with zero-range interactions, we had found that

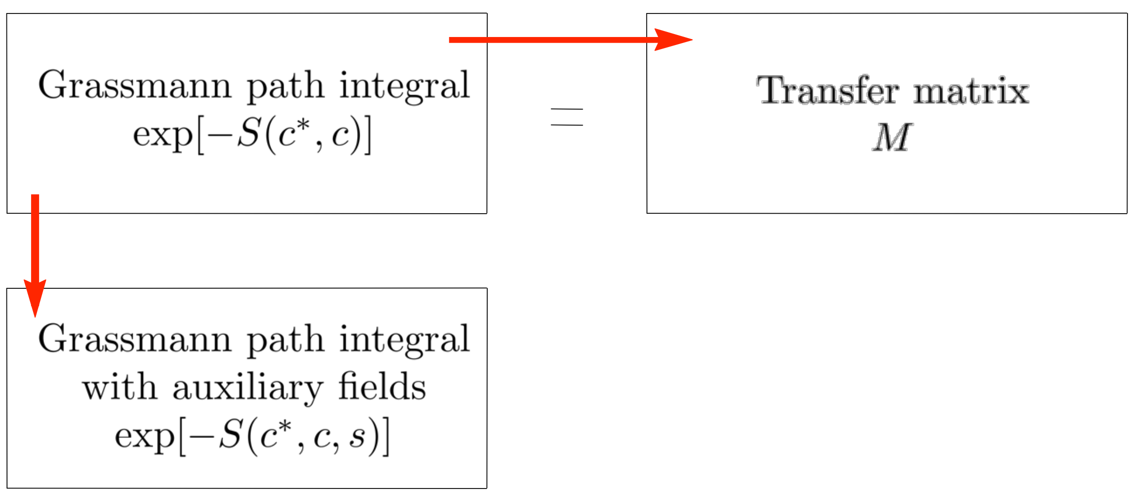
$$\mathcal{Z} = \int DcDc^* \exp\left[-S\left(c^*,c\right)\right] = Tr\left(M^{L_t}\right)$$

where

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

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

We now show the exact equivalence between the Grassmann path integral and the Grassmann path integral with auxiliary fields



Grassmann path integral with auxiliary fields

We can rewrite the same lattice Grassmann path integral using an auxiliary field

$$\mathcal{Z} = \prod_{\vec{n},n_t} \left[\int d_A s(\vec{n}, n_t)\right] \int DcDc^* \exp\left[-S_A\left(c^*, c, s\right)\right]$$

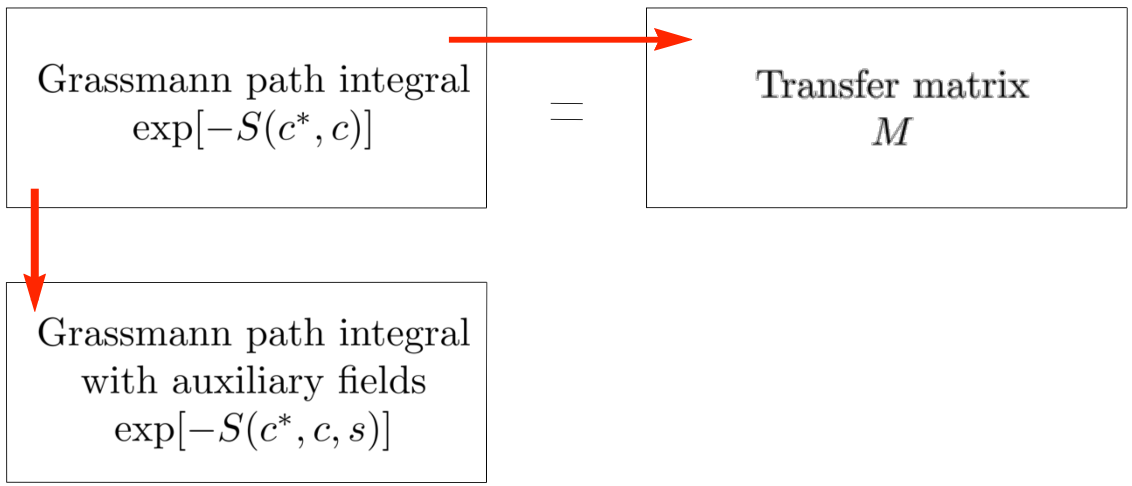
$$S_A\left(c^*, c, s\right) = S_{\text{free}}(c^*, c) - \sum_{\vec{n},n_t} A\left[s(\vec{n}, n_t)\right] \rho^{c^*,c}(\vec{n}, n_t)$$

where we have used the notation

$$\int d_A s(\vec{n}, n_t) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(\vec{n}, n_t) e^{-\frac{1}{2}s^2(\vec{n},n_t)}$$

$$A\left[s(\vec{n}, n_t)\right] \equiv \sqrt{-C\alpha_t}\, s(\vec{n}, n_t).$$

This demonstrates the exact equivalence of the following three lattice formulations for arbitrary lattice spacings:



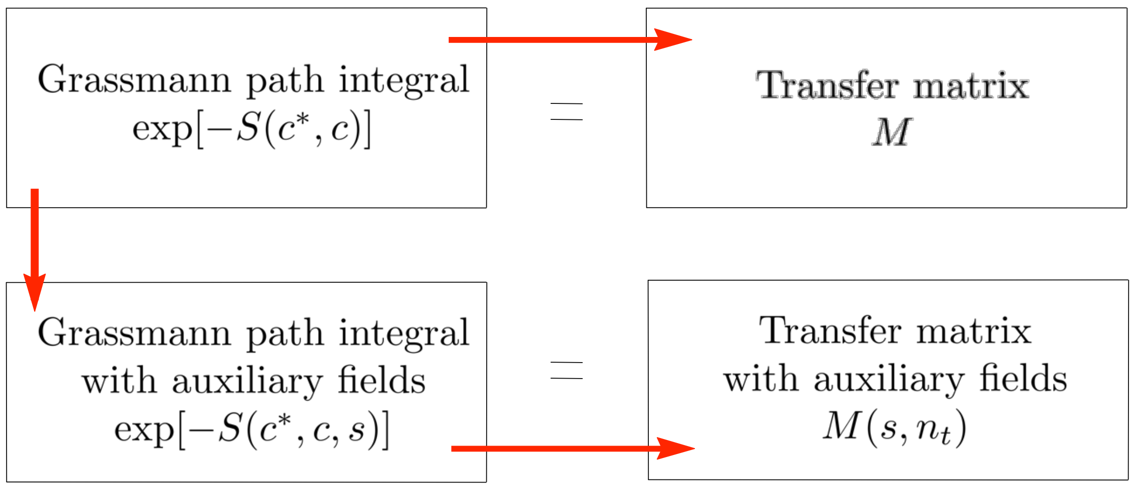
Transfer matrix operator with auxiliary fields

We use the equivalence of the Grassmann path integral and normal-ordered transfer matrix and apply it to the case of the auxiliary-field Grassmann path integral. We find

$$\mathcal{Z} = \prod_{\vec{n},n_t} \left[\int d_A s(\vec{n}, n_t)\right] Tr\left\{M_A(s, L_t - 1) \cdot \cdots \cdot M_A(s, 0)\right\}$$

$$M_A(s, n_t) =: \exp\left\{-H_{\text{free}}\alpha_t + \sum_{\vec{n}} A\left[s(\vec{n}, n_t)\right]\rho(\vec{n})\right\}:$$

This shows the exact equivalence of the following four lattice formulations for arbitrary lattice spacings:



Exercise

Prove the following formula for any set of functions f_{n_t},

$$\begin{aligned}
&\mathrm{Tr}\left\{: f_{L_t-1}(a^\dagger, a): \cdots : f_0(a^\dagger, a):\right\} \\
&\qquad = \int DcDc^* \exp\left\{\sum_{n_t=0}^{L_t-1} \sum_{\vec{n},i} c^*(n_t)\left[c(n_t) - c(n_t+1)\right]\right\} \\
&\qquad\qquad \times f_{L_t-1}\left[c^*(L_t-1), c(L_t-1)\right] \cdots f_0\left[c^*(0), c(0)\right]
\end{aligned}$$

where

$$c(L_t) = -c(0)$$

$$DcDc^* \equiv dc(L_t-1)dc^*(L_t-1)\cdots dc(0)dc^*(0)$$

Solution

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:

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

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

Let us define

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

We now have the following trace formula:

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

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

$$\sum_{i=0,1} f_{ii} = \sum_{i=0,1} \overrightarrow{\left(\frac{\partial}{\partial c^*}\right)}^i \tilde{f}(c^*,c) \overleftarrow{\left(\frac{\partial}{\partial c}\right)}^i \Bigg|_{c=c^*=0}$$
$$= \int dc dc^* (1 + c^* c) \tilde{f}(c^*, c)$$
$$= \int dc dc^* e^{c^* c} \tilde{f}(c^*, c)$$

We also note the following matrix product contraction formula:

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

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

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

And therefore we get

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

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

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

$$\begin{aligned}
&\mathrm{Tr}\left\{: f_{L_t-1}(a^\dagger, a): \cdots : f_0(a^\dagger, a):\right\} \\
&\quad = \sum_{i_0,\ldots,i_{L_t-1}=0,1} [f_{L_t-1}]_{i_0 i_{L_t-1}} [f_{L_t-2}]_{i_{L_t-1} i_{L_t-2}} \cdots [f_0]_{i_1 i_0} \\
&\quad\quad = \int DcDc^* \exp\left\{\sum_{n_t=0}^{L_t-1} \sum_{\vec{n},i} c^*(n_t)\left[c(n_t) - c(n_t+1)\right]\right\} \\
&\quad\quad\quad \times f_{L_t-1}\left[c^*(L_t-1), c(L_t-1)\right] \cdots f_0\left[c^*(0), c(0)\right]
\end{aligned}$$

where

$$c(L_t) = -c(0)$$