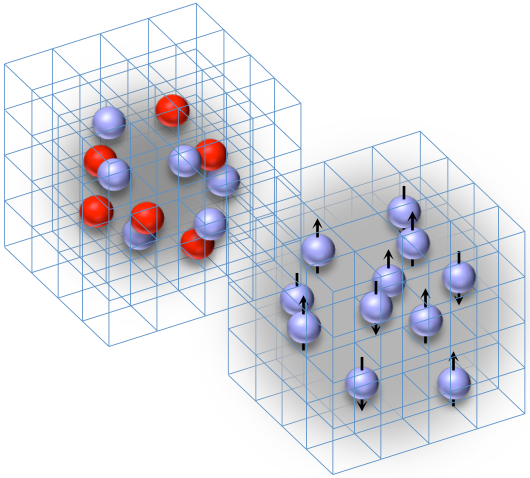
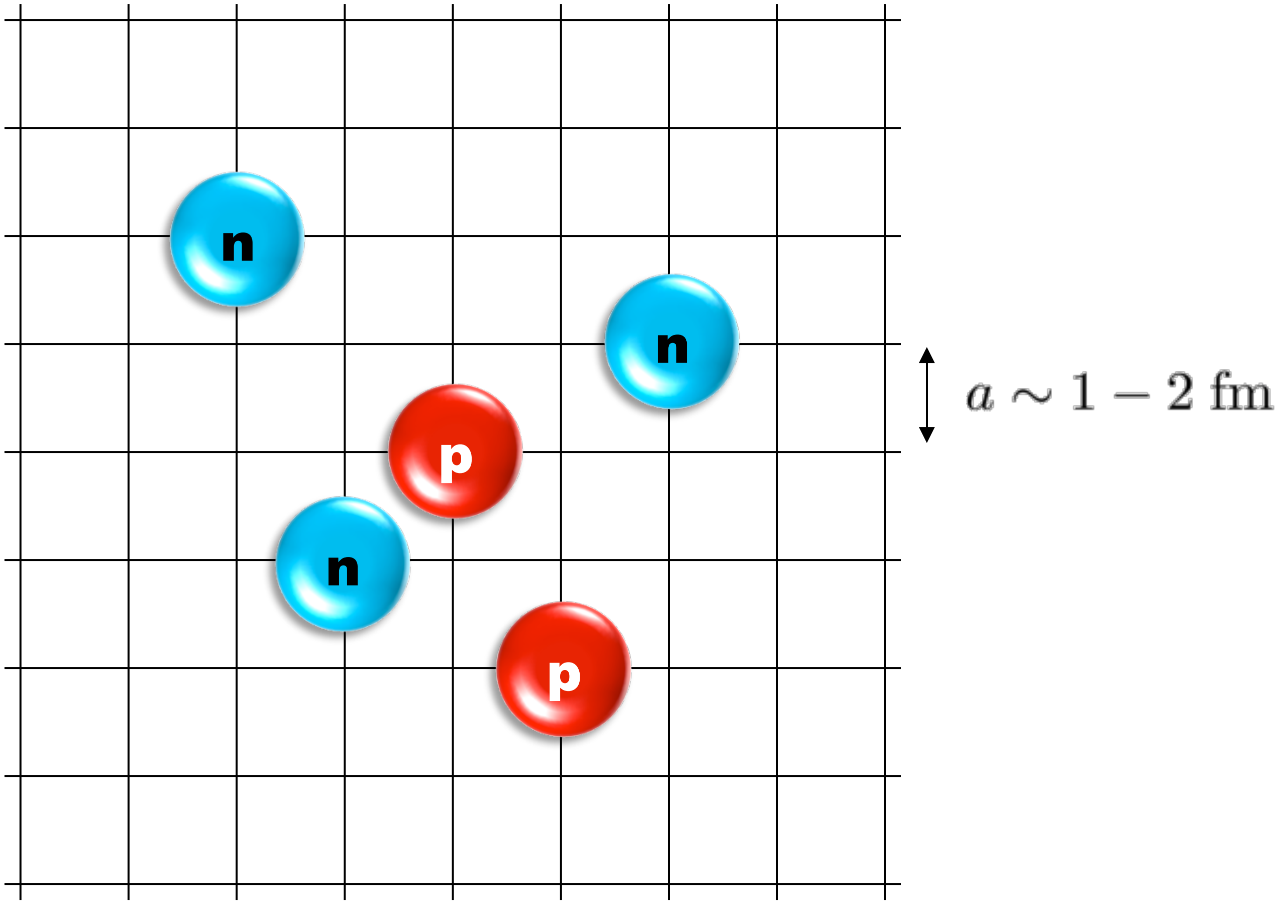
Lecture 17: Non-Relativistic Fermions

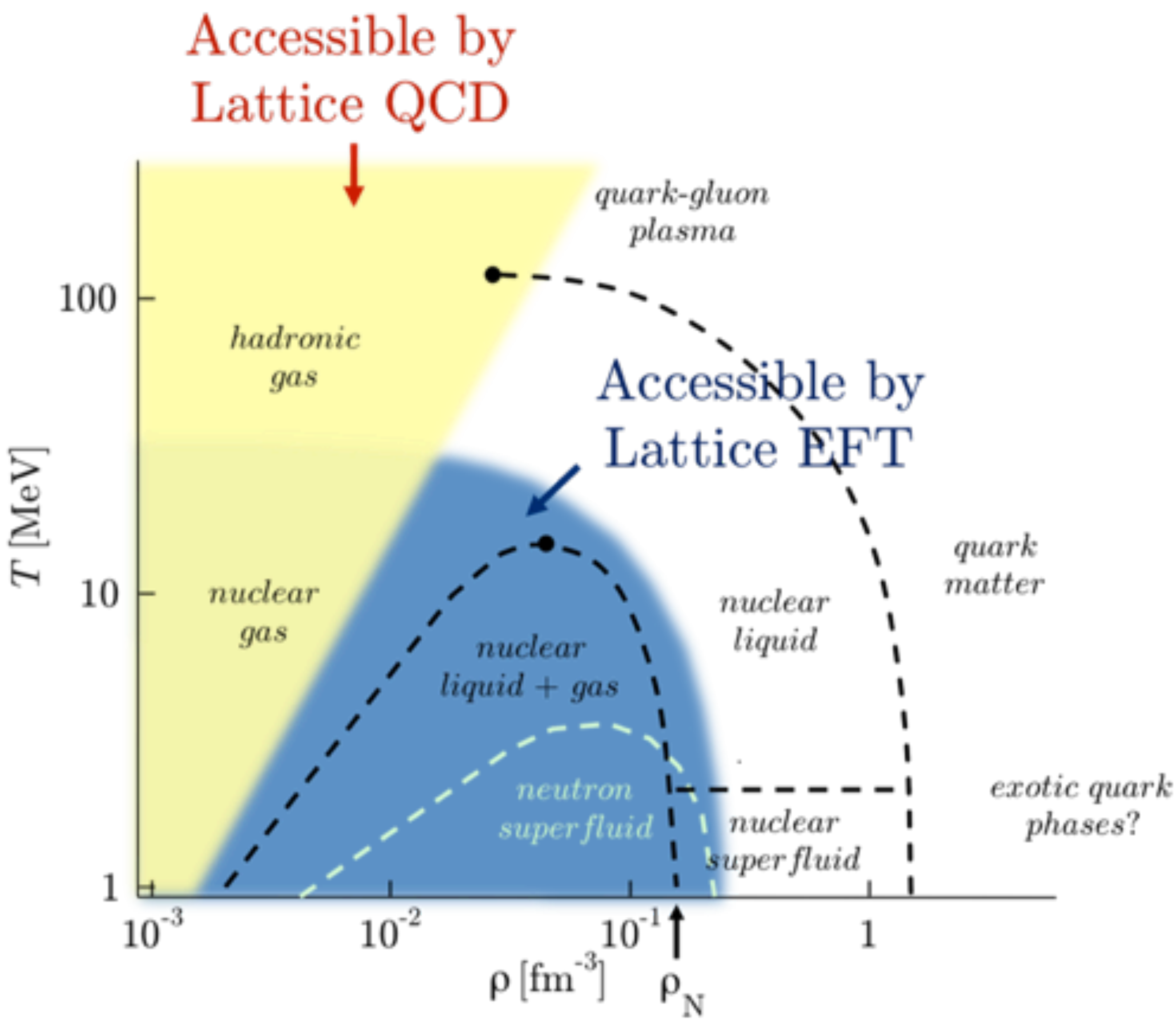
Dean Lee
Facility for Rare Isotope Beams
Michigan State University
Nuclear Lattice EFT Collaboration
July 25, 2019



ECT*
From Quarks and Gluons to Nuclear Forces and Structure

Nuclear lattice effective field theory

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1
10^{-3}
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ρ [fm^{-3}]
ρ_N

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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 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 sequential product of normal-ordered functions of the annihilation and creation operators.

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

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

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:

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

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

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

Putting everything together we can get an expression for the trace of a product of several matrices

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

in terms of Grassmann integrals involving functions

$$f_{L_t-1}(c^*(L_t-1), c(L_t-1)), f_{L_t-2}(c^*(L_t-2), c(L_t-2)), \cdots f_0(c^*(0), c(0))$$

These functions can involve coefficients that are also Grassmann variables. We will assume that every term has an even number of Grassmann variables.

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

$$= \int dc(0)dc^*(L_t-1)e^{c^*(L_t-1)c(0)}$$ (contraction and antiperiodic boundary)

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

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

$$\cdots$$

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

$$\cdot e^{c^*(0)c(0)} f_0(c^*(0), c(0))$$ (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

$$\mathrm{Tr}\left\{: f_{L_t-1}(a^\dagger, a) : \cdots : f_0(a^\dagger, a) :\right\}$$

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

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

$$\times f_{L_t-1}\left[c^*(L_t-1), c(L_t-1)\right] \cdots f_0\left[c^*(0), c(0)\right]$$

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

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

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

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

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

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

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

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

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

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

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

Homework for July 25

1. Prove this step from Lecture 17, Page 19:

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

Homework for July 25

2. Prove this step from Lecture 17, Page 19:

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

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

Homework for July 25

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

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

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

Homework for July 26

Write a code that expresses as a matrix, the lattice Hamiltonian for one free non-relativistic particle:

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

Find the energy spectrum of this matrix for a cubic periodic box of length 8 lattice units and mass m equal to 1 in lattice units.

Derive analytic expressions for these energies, and check that the first 33 energies agree with the analytic expressions for these energies.