

## Species doubling and transfer matrices for fermionic fields

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The transfer-matrix formalism for relating Hamiltonian quantum mechanics and Euclidean path integrals is discussed in the context of fermionic fields. Particular emphasis is placed on the extra fermionic species encountered with the naive discretization of time. When both particles and antiparticles are present, the Wilson projection-operator formalism arises naturally for the temporal coordinate. We discuss in detail how the Hilbert space must be enlarged to remove these projections.

### I. INTRODUCTION

Nonperturbative phenomena in field theory have been most extensively investigated via formulations in discrete space-time. Indeed, Monte Carlo simulations of Euclidean lattice gauge theory have given remarkable information on quark confinement and other aspects of hadronic physics.<sup>1</sup>

The inclusion of fermionic fields in lattice calculations has raised several interesting issues. One is how to treat anticommuting fields in numerical simulations. Existing algorithms are rather demanding on computer facilities; consequently, there is extensive ongoing exploration for better techniques. Another unresolved issue concerns the infamous doublings of fermionic species on a lattice. Some simple transcriptions of Dirac fields onto a lattice give rise to more fermionic species than naively anticipated, while schemes which eliminate these extra particles tend to complicate chiral symmetry. In particular, Wilson has proposed a simple formulation which avoids extra species by inserting projection operators into the naive lattice action.<sup>2</sup> These operators, however, mutilate chiral symmetry. They do, nonetheless, serve to generate the appropriate chiral anomaly in the continuum limit of the theory.<sup>3</sup>

Lattice gauge theories have been studied in both the original Euclidean formulation of Wilson<sup>4</sup> and the Hamiltonian formulation proposed by Kogut and Susskind.<sup>5</sup> The connection between these approaches appears via the transfer-matrix formalism, as discussed in some detail in Refs. 6 and 7. One purpose of the present paper is to expand on the fermionic part of those treatments. Reference 6 was nonrigorous in making smoothness assumptions on the anticommuting fields, while Ref. 7 showed the positivity of the transfer matrix only for fermions treated with the Wilson projection-operator technique. The extension of the treatment of Ref. 7 to the staggered fermions of Ref. 5 is discussed in Ref. 8.

Because of the doubling mentioned above, the simplest transcription of the Hamiltonian for Dirac fields to a  $(d-1)$ -dimensional space lattice and continuous time gives rise to  $2^{(d-1)}$  species. A transfer-matrix treatment relating a  $d$ -dimensional Euclidean theory to this Hamiltonian theory must, therefore, begin with less doubling than the "naive" transcription of Dirac fields to a Eu-

clidean lattice, which would give  $2^d$  species. We will see that the Wilson projection-operator formalism in the time direction arises quite naturally when one attempts to formulate such a transfer matrix. Indeed, with the projection operators in place one has a rather special case. Other formulations give rise to a transfer matrix operating in a larger Hilbert space containing the extra factor of 2 in the number of fermionic species.

To keep this paper reasonably self-contained, it has considerable repetition of material which already exists in the literature. References 9 and 10 are standard references on the formulation of fermions and path integrals. It is assumed that the reader has some familiarity with transfer matrices for bosonic fields, as discussed in Ref. 6.

Section II of this paper reviews the basic formulas for fermionic integrals as will be needed for the remainder of the paper. Section III discusses the Hilbert space of functions of anticommuting Grassmann variables. Section IV discusses the relation between operators in this space and functions of two arguments. For the transfer matrix these arguments represent the fields at two successive times. In Sec. V we consider a simple Hamiltonian and discuss the connection with path integrals. In Sec. VI we show how the Wilson action arises naturally for the time discretization when both particles and antiparticles are present. Section VII turns to the doubling problem and discusses the appearance of extra species when other actions are taken. Concluding remarks appear in Sec. VIII.

### II. REVIEW OF FERMIONIC INTEGRATION

In this section we briefly review fermionic integration and establish conventions for later use. We begin by considering a set  $\{\psi_i\}$  of anticommuting Grassmann variables

$$[\psi_i, \psi_j]_+ \equiv \psi_i \psi_j + \psi_j \psi_i = 0. \quad (2.1)$$

Generalizing complex conjugation to include these variables, we adopt the convention that corresponding to each  $\psi_i$ , we have another independent Grassmann variable  $\psi_i^*$ . Furthermore, we have

$$\begin{aligned} (\psi_i^*)^* &= \psi_i, \\ (\psi_1 \cdots \psi_n)^* &= \psi_n^* \cdots \psi_1^*. \end{aligned} \quad (2.2)$$

If we consider just a single variable  $\psi$ , a general function  $f(\psi)$  can be expanded with just two terms:

$$f(\psi) = f_0 + \psi f_1. \quad (2.3)$$

To define integration over an anticommuting variable, we wish to have the properties of linearity and invariance under a translation of variables. These are summarized in the axioms

$$\int d\psi (f(\psi)\alpha + g(\psi)\beta) = \left[ \int d\psi f(\psi) \right] \alpha + \left[ \int d\psi g(\psi) \right] \beta, \quad (2.4a)$$

$$\int d\psi f(\psi) = \int d\psi f(\psi + \psi'). \quad (2.4b)$$

This is enough to imply that, for the function in Eq. (2.2),

$$\int d\psi f(\psi) = K f_1, \quad (2.5)$$

where the normalization  $K$  is undetermined. We adopt the convention  $K = i$  so that

$$\begin{aligned} \int d\psi \psi &= i, \\ \int d\psi 1 &= 0, \\ \int d\psi^* d\psi \psi^* \psi &= 1. \end{aligned} \quad (2.6)$$

Note that for a multiplicative rescaling we have the relation

$$\int d\psi f(\psi a) = \left[ \int d\psi f(\psi) \right] a. \quad (2.7)$$

For integration over several anticommuting variables, we have

$$\int d\psi_1 \cdots d\psi_n \psi_1 \cdots \psi_n = i^n (-1)^{n(n-1)/2}. \quad (2.8)$$

The analog of Eq. (2.7) in this case is

$$\int (d\psi) f(M\psi) = |M| \int d\psi f(\psi), \quad (2.9)$$

where  $M$  is an arbitrary invertible matrix,  $|M|$  is its determinant, and  $(d\psi)$  denotes  $d\psi_1 \cdots d\psi_n$ . Note that Eq. (2.9) immediately implies the Mathews-Salam formula for a fermionic Gaussian integral:

$$\int (d\psi^* d\psi) e^{\psi^* M \psi} = |M|, \quad (2.10)$$

where

$$(d\psi^* d\psi) = d\psi_1^* d\psi_1 \cdots d\psi_n^* d\psi_n.$$

In addition to integration, it is sometimes useful to consider differentiation with respect to a Grassmann variable. This can be defined by the action on a constant function and an anticommutation relation

$$\frac{d}{d\psi} 1 = 0, \quad \left[ \frac{d}{d\psi}, \psi \right]_+ = 1. \quad (2.11)$$

Note the peculiar relation between integration and differentiation

$$\frac{d}{d\psi} f(\psi) = -i \int d\psi f(\psi). \quad (2.12)$$

### III. THE FERMIONIC HILBERT SPACE

The space of all functions of a set of Grassmann variables forms the Hilbert space on which our transfer matrices will act. We begin by considering just a single variable, in which case our space will be only two dimensional; i.e., there will be one fermionic state which is either occupied or not. Wishing to use a Dirac bra and ket notation, for any function there is a one-to-one correspondence with a ket state

$$f(\psi) \leftrightarrow |f\rangle. \quad (3.1)$$

We are pursuing an analogy with ordinary quantum mechanics with a commuting coordinate  $x$ , where one considers the correspondence between square integrable functions  $\phi(x)$  and quantum states  $|\phi\rangle$ .

We need a definition of an inner product for this space. This is somewhat more complicated than in the bosonic case where one has

$$\langle \phi | \phi' \rangle = \int dx \phi^*(x) \phi'(x). \quad (3.2)$$

If we just replace  $x$  and  $\phi(x)$  with  $\psi$  and  $f(\psi)$  in this relation, we would not obtain a positive norm. To proceed, it is useful to introduce the independent variable  $\psi^*$  and to relate each function  $f(\psi)$  to a second function

$$\bar{f}(\psi) = \int f(\psi)^* d\psi^* e^{\psi^* \psi} = i(f_0^* \psi - f_1^*). \quad (3.3)$$

Then an appropriate inner product between states corresponding to functions  $f(\psi)$  and  $g(\psi)$  is

$$\begin{aligned} \langle g | f \rangle &= \int \bar{g}(\psi) d\psi f(\psi) \\ &= \int [g(\psi)]^* d\psi^* e^{\psi^* \psi} d\psi f(\psi) \\ &= g_0^* f_0 + g_1^* f_1. \end{aligned} \quad (3.4)$$

For  $n$  variables this generalizes to

$$\begin{aligned} \langle g | f \rangle &= \int g(\psi)^* d\psi_n^* \cdots d\psi_1^* \\ &\quad \times \exp \left[ \sum \psi_i^* \psi_i \right] d\psi_1 \cdots d\psi_n f(\psi). \end{aligned} \quad (3.5)$$

We now introduce some simple operators in this space. In particular, we define an operator  $\hat{\psi}$  corresponding to the variable  $\psi$  via the relation

$$\psi f(\psi) \leftrightarrow \hat{\psi} |f\rangle. \quad (3.6)$$

This is the analog to defining the bosonic operator  $\hat{x}$  by  $\hat{x}|\phi\rangle$  being a state with wave function  $x\phi(x)$ . In terms of matrix elements,

$$\langle g | \hat{\psi} | f \rangle = \int g(\psi)^* d\psi^* e^{\psi^* \psi} d\psi \psi f(\psi). \quad (3.7)$$

While in the bosonic case  $\hat{x}$  is a Hermitian operator (at least if we consider wave functions that fall fast enough at infinity), this is not the case with the operator  $\hat{\psi}$  because of the distinction between  $\bar{f}$  and  $f$ . Instead, we have

$$\begin{aligned} \langle g | \hat{\psi}^\dagger | f \rangle &= (\langle f | \hat{\psi} | g \rangle)^* \\ &= \int g(\psi)^* \psi^* d\psi^* e^{\psi^* \psi} d\psi f(\psi) \\ &= \int \bar{g}(\psi) d\psi \frac{d}{d\psi} f(\psi). \end{aligned} \quad (3.8)$$

Indeed, it is easily verified that  $\hat{\psi}$  and  $\hat{\psi}^\dagger$  satisfy canonical fermion anticommutation relations

$$[\hat{\psi}, \hat{\psi}^\dagger]_+ = 1. \quad (3.9)$$

The operators  $\hat{\psi}$  and  $\hat{\psi}^\dagger$  are a complete set in the sense that any operator in the two-dimensional Hilbert space can be expressed in terms of them.

It is sometimes useful to have an explicit basis in mind for studying this space. A convenient one is to relate the function  $f(\psi) = \psi$  to a "vacuum" state  $|0\rangle$  and the function  $f(\psi) = 1$  to the "occupied" state  $|1\rangle$ . With these states we have

$$\begin{aligned} \hat{\psi}|1\rangle &= |0\rangle, \quad \hat{\psi}^\dagger|0\rangle = |1\rangle, \\ \hat{\psi}|0\rangle &= 0, \quad \hat{\psi}^\dagger|1\rangle = 0. \end{aligned} \quad (3.10)$$

Note some important differences between the above discussion and what occurs with commuting fields. In the latter case, to obtain an inner product the conjugate function  $\bar{\phi}(x)$  is simply the complex conjugate of  $\phi(x)$ . In particular, this implies that the operator  $\hat{x}$  corresponding to the real variable  $x$  is self-adjoint. To obtain a complete set of operators, one is forced to introduce something else, usually taken to be the conjugate momentum  $\hat{p}$  satisfying  $[\hat{p}, \hat{x}] = -i$ . In contrast, for fermions the conjugate momentum is simply the adjoint of the fundamental field.

#### IV. MORE OPERATORS

Given any function of two Grassmann fields  $A(\psi, \psi')$  we can define a corresponding operator  $\hat{A}$  in the quantum-mechanical Hilbert space. The action of the operator  $\hat{A}$  on the state  $|f\rangle$  corresponding to the function  $f(\psi)$  gives a state  $|g\rangle$  corresponding to the function

$$g(\psi) = \int A(\psi, \psi') d\psi' f(\psi'). \quad (4.1)$$

Although we will continue to write our equations in terms of a single degree of freedom, this and most of the following equations are immediately generalized to more variables.

The product of two operators is simple in this formalism; indeed, the function

$$C(\psi, \psi') = \int A(\psi, \psi'') d\psi'' B(\psi'', \psi') \quad (4.2)$$

corresponds to the operator

$$\hat{C} = \hat{A} \hat{B}. \quad (4.3)$$

In our notation, the trace of an operator takes the form

$$\text{Tr} \hat{A} = \int d\psi A(\psi, -\psi) = \int A(-\psi, \psi) d\psi. \quad (4.4)$$

The minus signs in this equation are one manifestation of the preference for antiperiodic boundary conditions with fermionic fields.

It is perhaps useful to consider some explicit operators for the case of a single degree of freedom, where only four functions form a complete set. We express the corresponding operators in terms of  $\hat{\psi}$  and  $\hat{\psi}^\dagger$  of the last section to obtain the relationships

$$\begin{aligned} A \leftrightarrow \hat{A}: \quad 1 &\leftrightarrow i\hat{\psi}^\dagger, \quad \psi \leftrightarrow i\hat{\psi}\hat{\psi}^\dagger, \\ \psi' &\leftrightarrow -i\hat{\psi}^\dagger\hat{\psi}, \quad \psi\psi' \leftrightarrow -i\hat{\psi}. \end{aligned} \quad (4.5)$$

Note the peculiar cross mapping of functions with an odd (even) number of Grassmann variables onto operators with an even (odd) number of fermionic fields. This is because of the Grassmann nature of  $d\psi'$  in Eq. (4.1).

An interesting specific case is the Grassmann generalization of the Dirac  $\delta$  function. This is defined by the relation

$$\int \delta(\psi, \psi') d\psi' f(\psi') = f(\psi). \quad (4.6)$$

For one degree of freedom, this function is

$$\delta(\psi, \psi') = -i(\psi - \psi'). \quad (4.7)$$

Introducing an auxiliary Grassmann variable  $\psi^*$ , we have the integral representation

$$\delta(\psi, \psi') = \int d\psi^* e^{\psi^*(\psi' - \psi)} = \int e^{-\psi^*\psi} d\psi^* e^{\psi^*\psi} \quad (4.8)$$

which looks somewhat reminiscent of the scalar formula

$$\delta(x - x') = \int e^{ip(x - x')} dp / 2\pi.$$

By our definitions, the operator corresponding to this function is simply the identity

$$\delta(\psi, \psi') \leftrightarrow \hat{I}. \quad (4.9)$$

As a preliminary example of a transfer matrix, consider the operator

$$\hat{T} = e^{-\epsilon \hat{\psi}^\dagger \hat{\psi}} = 1 + (e^{-\epsilon} - 1) \hat{\psi}^\dagger \hat{\psi}. \quad (4.10)$$

This is the quantum-mechanical operator generating a Euclidean time translation with a step  $\epsilon$  under Hamiltonian  $H = \hat{\psi}^\dagger \hat{\psi}$ . The function which corresponds to this is

$$T(\psi, \psi') = -i(\psi - e^{-\epsilon} \psi'). \quad (4.11)$$

To put this in a more manageable form, we introduce the auxiliary Grassmann variable  $\psi'^*$  as in Eq. (4.8) and write

$$T(\psi, \psi') = \int e^{\psi'^*(e^{-\epsilon}\psi - \psi')} d\psi'^*. \quad (4.12)$$

This may look more transparent if we rename  $\psi' = \psi_t$ ,  $\psi'^* = \psi_t^*$ , and  $\psi = \psi_{t+1}$ , while rewriting (4.12) in the form

$$T(\psi_{t+1}, \psi_t) = \int e^{-L} d\psi_t^*, \quad (4.13)$$

where

$$L = \psi_t^*(\psi_{t+1} - \psi_t) + (1 - e^{-\epsilon}) \psi_t^* \psi_t. \quad (4.14)$$

This is a discretization of the continuum Lagrangian density

$$L_c = \psi^* \partial_0 \psi + \epsilon \psi^* \psi. \quad (4.15)$$

Note that even though  $\hat{T}$  is Hermitian, the lattice derivative in Eq. (4.14) is defined in an asymmetric way under time reversal. In particular, while  $L$  contains a term  $\psi_t^* \psi_{t+1}$ , it does not contain  $\psi_{t+1}^* \psi_t$ . Indeed, because of the difference between  $f^*(\psi)$  and  $f(\psi)$ , to obtain the function corresponding to the adjoint of an operator requires more than just taking the complex conjugate of the

transpose. More precisely, if we adopt the standard definition of adjoint

$$\langle g | \hat{A}^\dagger | f \rangle = (\langle f | \hat{A} | g \rangle)^*, \quad (4.16)$$

then the function corresponding to  $\hat{A}^\dagger$  is

$$A^\dagger(\psi, \psi') = \int e^{-\psi^* \psi} d\psi^* (A(\psi', \psi))^* d\psi' e^{\psi^* \psi}. \quad (4.17)$$

One way to determine if a function  $A(\psi, \psi')$  corresponds to a Hermitian operator is to look at the transform

$$\mathcal{A}(\psi, \psi^*) = \int A(\psi, \psi') d\psi' e^{-\psi^* \psi}. \quad (4.18)$$

Then  $\hat{A} = \hat{A}^\dagger$  if

$$\mathcal{A}(\psi, \psi^*) = (\mathcal{A}(\psi^*, \psi))^* \quad (4.19)$$

using the conventions of Eq. (2.2). We note in passing that the treatment in Ref. 7 works directly with the functions  $\mathcal{A}(\psi, \psi^*)$ , inserting the factor of  $e^{-\psi^* \psi}$  from Eq. (4.18) into the formulas for products of operators.

Given an arbitrary function  $A(\psi, \psi')$ , it is useful to have a general formula for the operator  $\hat{A}$  in terms of our fundamental operator fields  $\hat{\psi}$  and  $\hat{\psi}^\dagger$ . The analogous formula for the bosonic case using the operators  $\hat{p}$  and  $\hat{x}$  is

$$\hat{A}(\hat{p}, \hat{x}) = \int d\Delta e^{i\hat{p}\Delta} A(\hat{x} + \Delta, \hat{x}). \quad (4.20)$$

For fermions the formula is quite similar except  $\hat{\psi}^\dagger$  replaces  $\hat{p}$  as the generator of translations in field space

$$e^{-\hat{\psi}^\dagger \psi} \hat{\psi} = (\hat{\psi} + \psi) e^{-\hat{\psi}^\dagger \psi}. \quad (4.21)$$

We give both normal-ordered and anti-normal-ordered forms

$$\hat{A} = \int d\psi e^{-\hat{\psi}^\dagger \psi} A(\psi - \hat{\psi}, -\hat{\psi}), \quad (4.22a)$$

$$\hat{A} = \int d\psi A(-\hat{\psi}, -\hat{\psi} - \psi) e^{-\hat{\psi}^\dagger \psi}. \quad (4.22b)$$

The Appendix contains an explicit derivation of these equations. We note in passing that the operator  $e^{-\hat{\psi}^\dagger \psi}$  appearing in these equations creates the fermionic coherent states used in Refs. 6 and 10. Several useful consequences of Eq. (4.22) are

$$A(\psi, \psi') = B(\psi) \Rightarrow \hat{A} = iB(\hat{\psi})\hat{\psi}^\dagger, \quad (4.23a)$$

$$A(\psi, \psi') = B(\psi') \Rightarrow \hat{A} = i\hat{\psi}^\dagger B(-\hat{\psi}), \quad (4.23b)$$

$$A(\psi, \psi') = \psi B(\psi, \psi') \Rightarrow \hat{A} = \hat{\psi} \hat{B}, \quad (4.23c)$$

$$A(\psi, \psi') = B(\psi, \psi') \psi' \Rightarrow \hat{A} = -\hat{B} \hat{\psi}. \quad (4.23d)$$

It is also useful to have formulas for the inverse problem: given an operator expressed in terms of  $\hat{\psi}$  and  $\hat{\psi}^\dagger$ , find the corresponding function. If the operator is in the form of a normal-ordered product  $A = \alpha(\hat{\psi}^\dagger)\beta(\hat{\psi})$ , then the corresponding function is

$$A(\psi, \psi') = \int \alpha(\psi^*)\beta(\psi') e^{\psi^*(\psi - \psi')} d\psi^*. \quad (4.24)$$

If the operator is anti-normal-ordered,  $A = \beta(\hat{\psi})\alpha(\hat{\psi}^\dagger)$  then we have

$$A(\psi, \psi') = \int \beta(\psi)\alpha(\psi^*) e^{\psi^*(\psi' - \psi)} d\psi^*. \quad (4.25)$$

## V. HAMILTONIANS AND TRANSFER MATRICES

With all this machinery in hand, we can now discuss simple Hamiltonians and the Euclidian actions which correspond to them. The transfer matrix as an operator translates a quantum-mechanical system a small step forward in Euclidian time. Thus if temporal dynamics is determined by a Hamiltonian operator  $H$ , we define the transfer matrix to be

$$\hat{T} = e^{-\epsilon H}, \quad (5.1)$$

where  $\epsilon$  is the step size. Conversely, given a lattice theory with a positive transfer matrix, this relation defines the corresponding Hamiltonian.

Given some transfer matrix  $\hat{T}$ , our general strategy is to find the function of fields at successive times which corresponds to this operator

$$T(\psi, \psi') \leftrightarrow \hat{T}. \quad (5.2)$$

We can then obtain the trace of the transfer matrix to a power  $N$  as a multiple integral over the anticommuting fields:

$$\text{Tr}(\hat{T}^N) = \int T(\psi_N, \psi_{N-1}) \times d\psi_{N-1} \cdots T(\psi_1, \psi_0) d\psi_0 |_{\psi_N = -\psi_0}. \quad (5.3)$$

If the integrand can be written in the form of a path integral over an exponentiated action, then we have obtained the action which corresponds to the original Hamiltonian.

Already in the previous section we considered the simple case of one degree of freedom with  $H = \hat{\psi}^\dagger \hat{\psi}$ . There we introduced the auxiliary field  $\psi^*$  in Eq. (4.12) in order to express the function  $T$  as an exponential of an action. Inserting that relation into Eq. (5.3) gives

$$\text{Tr}(T^N) = \int (d\psi^* d\psi) e^{-S} |_{\psi_N = -\psi_0}, \quad (5.4)$$

where

$$S = \sum_t [\psi_t^*(\psi_{t+1} - \psi_t) + (1 - e^{-\epsilon}) \psi_t^* \psi_t] \quad (5.5)$$

is the discretized action corresponding to this trivial Hamiltonian.

Actually, rather than path integrals themselves, the physically interesting quantities are Green's functions or correlation functions. In particular, consider creating a particle with  $\hat{\psi}^\dagger$  at some time, having it propagate  $n$  steps of size  $\epsilon$  forward in time, and then destroying it with the operator  $\hat{\psi}$ . This motivates looking at the following object:

$$\text{Tr}(\hat{\psi} \hat{T}^n \hat{\psi}^\dagger \hat{T}^{N-n}). \quad (5.6)$$

To express this in terms of a path integral, we note the correspondences

$$\hat{\psi} \hat{T} \leftrightarrow \psi T(\psi, \psi') = \int \psi e^{\psi^*(e^{-\epsilon}\psi - \psi')} d\psi^* \quad (5.7)$$

and

$$\hat{\psi}^\dagger \hat{T} \leftrightarrow \frac{d}{d\psi} T(\psi, \psi') = \int \psi^* e^{\psi^*(e^{-\epsilon}\psi - \psi')} d\psi^*. \quad (5.8)$$

This means that to obtain the propagator in Eq. (5.6), we

insert factors of  $\psi_n$  and  $\psi_{N-n-1}^*$  into the path integral in Eq. (5.4), with the result

$$\text{Tr}(\hat{\psi} \hat{T}^n \hat{\psi}^\dagger \hat{T}^{N-n}) = \int (d\psi^* d\psi) \psi_N \psi_{N-n-1}^* e^{-S} |_{\psi_N = -\psi_0} \quad (5.9)$$

This is valid for all  $n \geq 0$ . In general, the substitutions

$$\hat{\psi} \rightarrow \psi_t, \quad \hat{\psi}^\dagger \rightarrow \psi_{t-1}^* \quad (5.10)$$

give the path-integral representation for correlation functions.

One might worry about how to resolve the relations in (5.10) with the fact that  $\psi$  and  $\psi^*$  anticommute while  $\hat{\psi}$  and  $\hat{\psi}^\dagger$  satisfy the canonical anticommutation relations of Eq. (3.9). The consistency lies in the fact that while relating  $\hat{\psi}$  to  $\psi$  follows from Eq. (4.23c) and is quite general, Eq. (5.8), used to relate  $\hat{\psi}^\dagger$  to  $\psi^*$ , depends sensitively on the detailed form of  $T$ . Thus the substitutions of Eq. (5.10) are to be made only after the operators have been ordered such that all creation operators  $\hat{\psi}^\dagger$  lie directly to the left of factors of  $T$ .

### VI. ANTIPARTICLES AND WILSON PROJECTION OPERATORS

As noted above, the discretization of the continuum derivative connecting Eqs. (4.14) and (4.15) is asymmetric. Clearly it is somewhat a convention whether we use a forward or a backward definition of the lattice derivative. An interesting case occurs when we have both particles and antiparticles. Here it is quite natural to use different conventions for each.

To follow this idea in more detail, consider the Hilbert space generated by acting on a vacuum state with creation operators  $a^\dagger$  and  $b^\dagger$  for particles and antiparticles, respectively. In parallel with our earlier discussion, we relate this to the space of functions of two independent variables  $\psi$  and  $\chi^*$ . As before we related the variable  $\psi$  to the operator  $\hat{\psi}$ , here we relate

$$\psi \leftrightarrow a, \quad \chi^* \leftrightarrow b \quad (6.1)$$

The inner product between states takes the form

$$\langle g | f \rangle = \int g(\psi, \chi^*)^* d\psi^* d\chi e^{\psi^* \psi - \chi^* \chi} d\chi^* d\psi f(\psi, \chi^*) \quad (6.2)$$

Considering the Hamiltonian  $H = a^\dagger a + b^\dagger b$ , we want to find the function corresponding to the transfer matrix:

$$\hat{T} = \exp[-\epsilon(a^\dagger a + b^\dagger b)] \quad (6.3)$$

The generalization of Eq. (4.11) is

$$T(\psi, \chi^*; \psi', \chi'^*) = (\chi^* - e^{-\epsilon \chi'^*})(\psi - e^{-\epsilon \psi'}) \quad (6.4)$$

As in Eq. (4.12), we introduce the auxiliary variables  $\psi'^*$  and  $\chi'$  to rewrite Eq. (6.4) as

$$T(\psi, \chi^*; \psi', \chi'^*) = \int e^{-L} d\psi'^* d\chi' \quad (6.5)$$

where

$$L = \psi'^*(\psi - e^{-\epsilon \psi'}) - (\chi^* - e^{-\epsilon \chi'^*})\chi' \quad (6.6)$$

This can be written more compactly if we introduce two component vector Grassmann variables:

$$\eta = \begin{bmatrix} \psi \\ \chi \end{bmatrix}, \quad \bar{\eta} = (\psi^*, -\chi^*) \quad (6.7)$$

In this two-component space we define the projection operators

$$P_+ = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad P_- = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \quad (6.8)$$

Our lattice action now takes the form

$$L = -e^{-\epsilon} \bar{\eta} \eta + \bar{\eta}' P_+ \eta + \bar{\eta} P_- \eta' \quad (6.9)$$

We can introduce two-dimensional Dirac matrices to put this in a more familiar form. One possible convention is to take

$$\gamma_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \gamma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad (6.10)$$

$$\gamma_5 = \gamma_0 \gamma_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

in which case  $\bar{\eta} = \eta^* \gamma_0$  and Eq. (6.9) becomes

$$L = -e^{-\epsilon} \bar{\eta} \eta + \bar{\eta}' \frac{1}{2} (1 + \gamma_0) \eta + \bar{\eta} \frac{1}{2} (1 - \gamma_0) \eta' \quad (6.11)$$

Thus we see that the Wilson projection-operator formalism arises quite naturally for the treatment of the lattice time derivative.

Alternatively, we could use a representation of the Dirac matrices, where

$$\tilde{\gamma}_0 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \tilde{\gamma}_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad (6.12)$$

$$\tilde{\gamma}_5 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

This gives  $\bar{\eta} = \eta^* \tilde{\gamma}_0 \tilde{\gamma}_5$  and

$$P_\pm = \frac{1}{2} (1 \pm \tilde{\gamma}_0 \tilde{\gamma}_5) \quad (6.13)$$

Such a form was suggested in Ref. 11.

With an even number of degrees of freedom, this discussion is easily generalized to a Hamiltonian of the form

$$H = \hat{\psi}^\dagger M \hat{\psi} \quad (6.14)$$

where  $M$  is a Hermitian matrix. For example, the indices on  $M$  might include the particle momentum in a higher-dimensional spatial lattice. Keeping only terms to first order in  $\epsilon$  and using Wilson projections operators while symmetrizing between normal ordering and anti-normal-ordering, we consider the transfer operator

$$\hat{T} = 1 + \epsilon (\hat{\psi}_i^\dagger (P_+ M)_{ij} \hat{\psi}_j - \hat{\psi}_j (P_- M)_{ij} \hat{\psi}_i^\dagger) \quad (6.15)$$

where we adopt the convention  $P_\pm = \frac{1}{2} (1 \pm \gamma_0)$ . From this we can directly use Eqs. (4.24) and (4.25) to find the corresponding function

$$T(\psi, \psi') = \int d\chi e^{\chi(\psi' - \psi)} [1 + \epsilon(\chi P_+ M \psi' + \chi P_- M \psi)] . \quad \chi = \bar{\psi}_{t-1} P_+ - \bar{\psi}_t P_- . \quad (6.17)$$

We now rename  $\psi' = \psi_{t-1}$ ,  $\psi = \psi_t$ , and

Continuing to work to lowest order in  $\epsilon$ , we make these substitutions and write

$$T(\psi_t, \psi_{t-1}) = \int d\chi \exp[-\bar{\psi}_{t-1} P_+ \psi_t - \bar{\psi}_t P_- \psi_{t-1} + \bar{\psi}_{t-1} P_+ \psi_{t-1} + \bar{\psi}_t P_- \psi_t + \epsilon(\bar{\psi}_{t-1} P_+ M \psi_{t-1} - \bar{\psi}_t P_- M \psi_t)] . \quad (6.18)$$

If we now construct the path integral

$$\text{Tr} T^N = \int (d\bar{\psi} d\psi) e^{-S} \quad (6.19)$$

terms involving successive times combine and we obtain the action

$$S = \sum_t (\bar{\psi}_{t-1} P_+ \psi_t + \bar{\psi}_t P_- \psi_{t-1} - \bar{\psi}_t \psi_t - \epsilon \bar{\psi}_t \gamma_0 M \psi_t) . \quad (6.20)$$

As one final comment in this section, consider the analog of Eqs. (5.10), which provide the machinery to construct correlation functions. The peculiar renaming in Eq. (6.17) introduces a temporal splitting when creation operators are considered. In particular, using the relation  $\hat{\psi}^\dagger \hat{T} \rightarrow (d/d\psi) T$  we obtain the correspondence

$$\hat{\psi}^\dagger \rightarrow \chi(1 - \epsilon P_- M) + O(\epsilon^2) \\ = \bar{\psi}_{t-1} P_+ - \bar{\psi}_t P_- (1 - \epsilon M) + O(\epsilon^2) . \quad (6.21)$$

Operators such as conserved charges in the Hamiltonian formalism thus acquire a somewhat complicated form when considered in a Euclidian path integral. For example, consider some current  $\hat{J} = \hat{\psi}^\dagger \Gamma \hat{\psi}$  at time  $t$ . Here  $\Gamma$  represents some combination of Dirac matrices. This operator corresponds to inserting into the path integral a factor of

$$J_t = \bar{\psi}_{t-1} P_+ \Gamma \psi_t - \bar{\psi}_t P_- (1 - \epsilon M) \Gamma \psi_t + \text{Tr} \Gamma + O(\epsilon^2) . \quad (6.22)$$

The  $\text{Tr} \Gamma$  term arises from reordering  $\hat{J}$  to put  $\hat{\psi}^\dagger$  to the right. This splitting of currents in the path integral can also be observed directly from symmetry considerations in the path integral.<sup>3</sup> The point here is that this complex relation may obscure the symmetries of the original Hamiltonian.

## VII. SPECIES DOUBLING

We now return to the example of a single fermion as discussed in Eqs. (4.10)–(4.15). In particular, we wish to discuss how the necessity of introducing the auxiliary extra variable  $\psi^*$  is indicative of the doubling problem. Indeed, having both  $\psi$  and  $\psi^*$  as variables at any given time suggests that we should consider the Hilbert space of functions of both. This, however, has twice as many states per degree of freedom than considered previously. For the special case of the action in Eq. (4.14) it is un-

necessary to look at this larger space, but for an arbitrary action one would be forced into such a doubling. To study this further, it is instructive to generalize the action density of Eq. (4.14) to

$$L = (1 - \alpha) [\psi_t^* (\psi_{t+1} - \psi_t) + (1 - e^{-\epsilon}) \psi_t^* \psi_t] \\ - \alpha [(\psi_{t+1}^* - \psi_t^*) \psi_t + (1 - e^{-\epsilon}) \psi_t^* \psi_t] . \quad (7.1)$$

Exponentiating this action, we consider the function

$$T(\psi^*, \psi; \psi'^*, \psi') = \exp[(1 - \alpha) \psi'^* \psi - \alpha \psi^* \psi' \\ - (1 - 2\alpha) e^{-\epsilon} \psi'^* \psi'] . \quad (7.2)$$

When the parameter  $\alpha$  goes to zero we obtain the action used in Eq. (4.14), while when  $\alpha$  goes to unity we have the action used for the antiparticle in Eq. (6.6), with  $\chi$  replaced by  $\psi$ . In the former case  $\psi^*$  was an auxiliary variable and we worked in the Hilbert space of functions of  $\psi$ , while in the latter  $\psi$  was the auxiliary variable and our states corresponded to functions of  $\psi^*$ . We now consider this interpolating action in the larger Hilbert space of functions of both  $\psi$  and  $\psi^*$ .

Going to a Hilbert space as in Sec. II, we relate a state  $|f\rangle$  with any function  $f(\psi, \psi^*)$ . The overlap of such states is

$$\langle g | f \rangle = \int g(\psi, \psi^*)^* d\psi^* d\psi e^{\psi^* \psi - \psi'^* \psi'} \\ \times d\psi'^* d\psi' f(\psi', \psi'^*) . \quad (7.3)$$

This equation is the same as Eq. (6.2) after some minor renaming of variables. In analogy with Eq. (3.6), we now define operators  $a$  and  $b$  corresponding to  $\psi$  and  $\psi^*$ , respectively. In the Appendix we derive the analog of Eq. (4.22):

$$\hat{A} = \int d\psi^* d\psi e^{a^\dagger \psi - \psi^* b^\dagger} A(\psi + a, \psi^* + b; a, b) . \quad (7.4)$$

Using this we obtain the operator corresponding to the function in Eq. (7.2):

$$\hat{T} = a^\dagger b^\dagger + \alpha(1 - \alpha) b a - (1 - \alpha) b^\dagger b e^{-\epsilon a^\dagger a} \\ + \alpha a^\dagger a e^{-\epsilon b^\dagger b} . \quad (7.5)$$

Observe that  $\hat{T}$  is not Hermitian. We can, however, relate it to a Hermitian operator by a simple similarity transformation which rescales the various states. This transformation is not unique; to preserve the  $\alpha \leftrightarrow (1 - \alpha)$  symmetry, we consider

$$G = \exp[-\frac{1}{2} a^\dagger a \ln(1 - \alpha) - \frac{1}{2} b^\dagger b \ln \alpha] . \quad (7.6)$$

This has the properties

$$\begin{aligned}
G^\dagger &= G, \\
G^{-1}aG &= (1-\alpha)^{-1/2}a, \\
G^{-1}bG &= \alpha^{-1/2}b, \\
G^{-1}a^\dagger G &= (1-\alpha)^{1/2}a^\dagger, \\
G^{-1}b^\dagger G &= \alpha^{1/2}b^\dagger.
\end{aligned} \tag{7.7}$$

Thus we have

$$\begin{aligned}
\tilde{T} &= G^{-1} \hat{T} G \\
&= [\alpha(1-\alpha)]^{1/2} (a^\dagger b^\dagger + ba) \\
&\quad - (1-\alpha) b^\dagger b e^{-\epsilon a^\dagger a} + \alpha a^\dagger a e^{-\epsilon b^\dagger b}
\end{aligned} \tag{7.8}$$

which is indeed a self-adjoint quantity. Of course, since  $\hat{T}$  and  $\tilde{T}$  differ only by a similarity transformation,  $\text{Tr}(\hat{T}^N) = \text{Tr}(\tilde{T}^N)$ . Note that as the parameter  $\alpha$  goes to either zero or one,  $\tilde{T}$  factorizes with either  $a$ - or  $b$ -type particles becoming trivially projected onto occupied states. For other values of  $\alpha$ , however, we must consider the full space containing both  $a$ - and  $b$ -type particles.

Note that for  $\alpha$  between 0 and 1,  $\tilde{T}$  is not a positive operator. This, however, is not a serious problem in defining a Hamiltonian as we can consider the square of  $\tilde{T}$  as generating a step of size  $2\epsilon$  forward in time. This is also done in the treatments of Refs. 8 and 11.

Rather than introducing the above similarity transformation, we could obtain a self-adjoint transfer matrix by replacing Eq. (3.4) with a rescaled overlap for our Hilbert space

$$\begin{aligned}
(g, f) &\equiv \int g(\psi, \psi^*)^* d\psi^* d\psi \\
&\quad \times \exp[(1-\alpha)\psi^* \psi' - \alpha\psi'^* \psi] \\
&\quad \times d\psi'^* d\psi' f(\psi', \psi'^*) \\
&= \langle g | G^{-2} | f \rangle.
\end{aligned} \tag{7.9}$$

Using this overlap, we can define a new "adjoint" operation under which  $\hat{T}$  is indeed invariant:

$$(g, \hat{T}^{(A)} f) \equiv (f, \hat{T} g)^* = (g, \hat{T} f). \tag{7.10}$$

As the parameter  $\alpha$  goes to zero, the operator  $G^{-2}$  is singular, annihilating states containing  $b$  particles. Such states will then have zero length under the rescaled norm. In the constructive formalism of Ref. 11, there is a step where zero-norm states are divided out to obtain the Hilbert space. The number of states thus removed suddenly increases as  $\alpha$  becomes zero and the extra species are eliminated.

## VIII. CONCLUDING REMARKS

We have set up a formalism for relating fermionic Hamiltonians with the corresponding path integrals. We have ignored couplings to bosonic fields, which could be easily added as in Refs. 6 and 7. We find that the transfer-matrix approach naturally gives rise to the Wilson projection-operator formalism for time derivatives. For this to be consistent with the symmetries of the Hamiltonian, the corresponding currents in the path integral receive a point splitting which also involves the projection operators. Thus a chiral symmetry of the original Hamiltonian may become obscure in the path integral.

One remaining question is how should one treat space derivatives. Clearly, hypercubic symmetry is simplest if they also carry projection operators. In this case, however, chiral symmetries will be broken already at the Hamiltonian level. Monte Carlo calculations also support the lack of any hidden continuous chiral symmetry in the Wilson formalism.

Our discussion shows that asymmetric definitions of time derivatives do not necessarily lead to non-Hermitian transfer matrices. Indeed, the discussion suggests that an asymmetric action may be necessary to treat self-conjugate particles or to give chiral couplings to fermions. This latter point deserves further study in view of possible relevance to treating weak interactions with lattice methods.

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## APPENDIX

In this appendix we derive the formulas in Eqs. (4.22) and (7.4) for finding the operators which correspond to a given function. Beginning with the single degree of freedom case, we consider a function  $A(\psi, \psi')$ . A general matrix element of the corresponding operator is

$$\langle f | \hat{A} | g \rangle = \int f(\psi_1)^* d\psi_1^* e^{\psi_1^* \psi_1} d\psi_1 A(\psi_1, \psi_2) d\psi_2 g(\psi_2). \tag{A1}$$

We now use the axiom of invariance of fermionic integration under shifts, Eq. (2.4a), to replace  $\psi_1$  with  $\psi_1 + \psi_2$  in the integrand

$$\begin{aligned}
\langle f | \hat{A} | g \rangle &= \int f(\psi_1)^* d\psi_1^* e^{\psi_1^* (\psi_1 + \psi_2)} d\psi_1 \\
&\quad \times A(\psi_1 + \psi_2, \psi_2) d\psi_2 g(\psi_2).
\end{aligned} \tag{A2}$$

Rearranging, we obtain

$$\langle f | \hat{A} | g \rangle = \int f(\psi_1)^* d\psi_1^* e^{\psi_1^* \psi_2} \left[ \int d\psi_1 e^{\psi_1^* \psi_1} A(\psi_1 + \psi_2, \psi_2) \right] d\psi_2 g(\psi_2). \tag{A3}$$

From the definitions of the operators  $\hat{\psi}$  and  $\hat{\psi}^\dagger$ , we see that  $\psi_2$  in the inner set of small parentheses corresponds to  $-\hat{\psi}$  and  $\psi_1^*$  corresponds to  $-\hat{\psi}^\dagger$ . Thus we read off Eq. (4.22a):

$$\hat{A} = \int d\psi e^{-\hat{\psi}^\dagger \psi} A(\psi - \hat{\psi}, -\hat{\psi}). \tag{4.22a}$$

In general, the minus signs in this equation will become  $-1$  to the number of fermionic species being considered. Equation (4.22b) directly follows from this equation and (4.21).

The derivation of Eq. (7.4) proceeds essentially identically. We have

$$\langle f | \hat{A} | g \rangle = \int f(\psi_1, \psi_1^*)^* d\psi_1^* d\psi_1 e^{\psi_1^* \psi_2 - \psi_2^* \psi_1} d\psi_2^* d\psi_2 A(\psi_2, \psi_2^*; \psi_3, \psi_3^*) d\psi_3^* d\psi_3 g(\psi_3, \psi_3^*) . \quad (\text{A4})$$

Shifting the  $\psi_2$  and  $\psi_2^*$  integrals, we find

$$\begin{aligned} \langle f | \hat{A} | g \rangle &= \int f(\psi_1, \psi_1^*)^* d\psi_1^* d\psi_1 e^{\psi_1^* \psi_3 - \psi_3^* \psi_1} \\ &\quad \times \left[ \int d\psi_2^* d\psi_2 e^{\psi_1^* \psi_2 - \psi_2^* \psi_1} A(\psi_2 + \psi_3, \psi_2^* + \psi_3^*; \psi_3, \psi_3^*) \right] d\psi_3^* d\psi_3 g(\psi_3, \psi_3^*) \end{aligned} \quad (\text{A5})$$

from which we read off Eq. (7.4).

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