Algebra of Conserved Generators and Statistical Ensembles in Generalized Quantum Dynamics *

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Abstract: We study here the algebraic structure of the conserved generators from which the microcanonical and canonical ensembles are constructed on an underlying generalized quantum dynamics, and the flows they induce on the phase space. We also discuss briefly the structure of the microcanonical and canonical ensembles.

* Presented as a talk by the second author at the Workshop on Algebraic Approaches to Quantum Dynamics, May 7-12, 1996, at the Fields Institute for Research in Mathematical Sciences, Toronto, Ontario, Canada.

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1. Introduction

It has recently been shown\(^1\), by application of statistical mechanical methods to determine the canonical ensemble governing the equilibrium distribution of operator initial values, that complex quantum field theory can emerge as a statistical approximation to an underlying generalized quantum dynamics.\(^2,3\) This result was obtained by an argument based on a Ward identity analogous to the equipartition theorem of classical statistical mechanics.\(^1\) In the following, we describe some features of generalized quantum dynamics and the motivation for its development. We then describe how the equilibrium ensembles are constructed, and briefly review the emergence of the usual complex quantum field theory in the ensemble average.

The field variables associated with a hypercomplex quantum theory, such as quaternionic quantum mechanics, form an essentially non-commutative set of functions, even when they are not second-quantized. The construction of a dynamical theory then requires a generalized structure, which is the main subject of our discussion here. To understand why this is so, consider the Heisenberg picture of a scalar field.\(^3\) The generator of evolution in time is taken as an anti-self-adjoint operator, since there is, in general, no natural complex unit to extract a self-adjoint operator from the representation of a one-parameter unitary group. The Heisenberg picture for a quaternionic field of the form

\[ \phi(x) = \sum_{A=0}^{3} \phi_A e_A, \]  

where \(e_0 = 1\) and \(e_1, e_2, e_3\) are the quaternionic units satisfying the cyclic relations

\[ e_1 e_2 = e_3, \quad e_2^2 = -1, \quad A = 1, 2, 3, \]  

is given by

\[ \phi_{H}(x, t) = e^{\hat{H}t} \phi(x) e^{-\hat{H}t} = \phi_0(x, t) + \sum_{A=1}^{3} \phi_{AH}(x, t) e_A(t), \]  

where the \(\{\phi_{AH}(x, t)\}\) are kinematically independent, i.e., the commutation relations are the same as the Schrödinger picture fields. However, if we expand over the original set of quaternionic units \(\{e_A\}\) on the components defined by

\[ \phi_{H}(x, t) = \sum_{A=0}^{3} \phi_{H}(x, t)_A e_A, \]  

then the \(\{\phi_{H}(x, t)_A\}\) are not kinematically independent. As an illustrative example, consider the simple case in which \(\hat{H}\) is some real valued operator multiplied by \(e_1\). Since

\[
\begin{align*}
e_{1H}(t) &= e_1 \\
e_{2H}(t) &= e^{\hat{H}t} e_2 e^{-\hat{H}t} = e^{2\hat{H}t} e_2 \\
e_{3H}(t) &= e^{\hat{H}t} e_3 e^{-\hat{H}t} = e^{2\hat{H}t} e_3,
\end{align*}
\]

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the coefficients of the constant \{e_A\} are

\[
\begin{align*}
\phi_H(x, t)_1 &= \phi_{1H}(x, t) \\
\phi_H(x, t)_2 &= \phi_{2H}(x, t)e^{2\tilde{H}t} \\
\phi_H(x, t)_3 &= \phi_{3H}(x, t)e^{2\tilde{H}t}.
\end{align*}
\]

Due to the presence of the additional factor containing \(\tilde{H}\), the commutation relations are not the same as those of the Schrödinger fields, and, in fact,

\[
[\phi_H(x, t)_A, \phi_H(x', t)_B] \neq 0. \tag{1.7}
\]

The same result is true for gauge fields of the form \(B_\mu = \sum B_{\mu A}e_A\). A similar structure was found in the studies of ref. 4, a program concerned with the static limit of generalized non-Abelian gauge theories. In order to construct a c-number action for theories of this type, the notion of a \textit{total trace} was introduced\(^2\,^3\), where both the quantum state and algebraic representation indices are summed over in the trace. As we shall see in the next section, one can define a total trace Lagrangian and Hamiltonian over an underlying phase space of quantum fields which results in a symplectic dynamics with many of the properties of classical mechanics. We shall the describe the flows induced by an important class of conserved operators, and show how a statistical mechanics can be constructed on the phase space of the underlying quantum fields.

### 2. Generalized quantum dynamics

Generalized quantum dynamics\(^2\,^3\) is an analytic mechanics on a symplectic set of operator valued variables, forming an operator valued phase space \(S\). These variables are defined as the set of linear transformations\(^\dagger\) on an underlying real, complex, or quaternionic Hilbert space (Hilbert module), for which the postulates of a real, complex, or quaternionic quantum mechanics are satisfied\(^3\,^5\,^6\,^7\,^8\). The dynamical (generalized Heisenberg) evolution, or flow, of this phase space is generated by the total trace Hamiltonian \(H = \text{Tr}H\), where

\[
\begin{align*}
\text{Tr}O &= \text{Re}\text{Tr}(-1)^F O \\
&= \text{Re} \sum_n \langle n|(-1)^F O|n\rangle, \tag{2.1}
\end{align*}
\]

\(H\) is a function of the operators \(\{q_r(t)\}, \{p_r(t)\}, \ r = 1, 2, \ldots, N\) (realized as a sum of monomials, or a limit of a sequence of such sums; in the general case of local noncommuting fields, the index \(r\) contains continuous variables), and \((-1)^F\) is a grading operator with eigenvalue \(1(-1)\) for states in the boson (fermion) sector of the Hilbert space. Operators are called bosonic or fermionic in type if they commute or anticommute, respectively, with \((-1)^F\); for each \(r\), \(p_r\) and \(q_r\) are of the same type.

The derivative of a total trace functional with respect to some operator variation is defined with the help of the cyclic property of the \text{Tr} operation. The variation of any

\(^\dagger\) In general, local (noncommuting) quantum fields.
monomial $O$ consists of terms of the form $O_L \delta x_r O_R$, for $x_r$ one of the $\{q_r\}, \{p_r\}$, which, under the $Tr$ operation, can be brought to the form

$$\delta O = \delta \text{Tr} O = \pm \text{Tr} O R L \delta x_r,$$

so that sums and limits of sums of such monomials permit the construction of

$$\delta O = \text{Tr} \sum_r \frac{\delta O}{\delta x_r} \delta x_r, \quad (2.2)$$

uniquely defining $\delta O/\delta x_r$.

Assuming the existence of a total trace Lagrangian$^{2,3}$ $L = L(\{q_r\}, \{\dot{q}_r\})$, the variation of the total trace action

$$S = \int_\infty^{-\infty} L(\{q_r\}, \{\dot{q}_r\}) dt \quad (2.3)$$

results in the operator Euler-Lagrange equations

$$\frac{\delta L}{\delta q_r} - \frac{d}{dt} \frac{\delta L}{\delta \dot{q}_r} = 0. \quad (2.4)$$

As in classical mechanics, the total trace Hamiltonian is defined as a Legendre transform,

$$H = \text{Tr} \sum_r p_r \dot{q}_r - L, \quad (2.5)$$

where

$$p_r = \frac{\delta L}{\delta \dot{q}_r}. \quad (2.6)$$

It then follows from (2.4) that

$$\frac{\delta H}{\delta q_r} = -\dot{p}_r \quad \frac{\delta H}{\delta p_r} = \epsilon_r \dot{q}_r, \quad (2.7)$$

where $\epsilon_r = 1(-1)$ according to whether $p_r, q_r$ are of bosonic (fermionic) type.

Defining the generalized Poisson bracket

$$\{A, B\} = \text{Tr} \sum_r \epsilon_r \left( \frac{\delta A}{\delta q_r} \frac{\delta B}{\delta p_r} - \frac{\delta B}{\delta q_r} \frac{\delta A}{\delta p_r} \right), \quad (2.8a)$$

one sees that

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \{A, H\}. \quad (2.8b)$$

Conversely, if we define

$$x_s(\eta) = \text{Tr}(\eta x_s), \quad (2.9a)$$
for $\eta$ an arbitrary, constant operator (of the same type as $x_s$, which denotes here $q_s$ or $p_s$), then
\[
\frac{dx_s(\eta)}{dt} = \text{Tr} \sum_r \epsilon_r \left( \frac{\delta x_s(\eta)}{\delta q_r} \frac{\delta H}{\delta p_r} - \frac{\delta H}{\delta q_r} \frac{\delta x_s(\eta)}{\delta p_r} \right),
\]
and comparing the coefficients of $\eta$ on both sides, one obtains the Hamilton equations (2.7) as a consequence of the Poisson bracket relation (2.8b).

The Jacobi identity is satisfied by the Poisson bracket of (2.8a), and hence the total trace functionals have many of the properties of the corresponding quantities in classical mechanics. In particular, canonical transformations take the form
\[
\delta x_s(\eta) = \{x_s(\eta), G\},
\]
which implies that
\[
\delta p_r = -\frac{\delta G}{\delta q_r}, \quad \delta q_r = \epsilon_r \frac{\delta G}{\delta p_r},
\]
with the generator $G$ any total trace functional constructed from the operator phase space variables. Time evolution then corresponds to the special case $G = H dt$.

3. Flows and algebras associated with conserved operators

The operator
\[
\hat{C} = \sum_r (\epsilon_r q_r p_r - p_r q_r)
\]
\[
= \sum_{r,B} [q_r, p_r] - \sum_{r,F} \{q_r, p_r\},
\]
where the sums are over bosonic and fermionic pairs, respectively, is conserved under the evolution (2.7) induced by the total trace Hamiltonian. When the equations of motion induced by the Lagrangian $L$ coincide with those induced by the ungraded total trace of the same Lagrangian (there are many models which have this property),
\[
\hat{L} = \text{Re} \text{Tr} L,
\]
without the factor $(-1)^F$, the corresponding ungraded total trace Hamiltonian $\hat{H}$ is conserved; it may therefore be included as a constraint functional in the canonical ensemble, along with the new conserved operator
\[
\hat{C} = \sum_r [q_r, p_r]
\]
\[
= \sum_{r,B} [q_r, p_r] + \sum_{r,F} [q_r, p_r].
\]

We now study the action of general total trace functionals projected from $\hat{C}$ and $\hat{C}$ as generators of canonical transformations on the phase space. We first remark that it was
pointed out in ref. 1 that a canonical generator of unitary transformations on the basis of the underlying Hilbert space has the form

\[ G_{\tilde{f}} = -\text{Tr} \sum_r [\tilde{f}, p_r] q_r, \]  

(3.3)

where \( \tilde{f} \) is bosonic. Using (3.1) and the cyclic properties of \( \text{Tr} \), one sees that

\[ G_{\tilde{f}} = -\text{Tr} \tilde{f} \sum_r (p_r q_r - \epsilon_r q_r p_r) \]

(3.4)

\[ = \text{Tr} \tilde{f} C. \]

We thus see that the conserved operator \( \tilde{C} \) has the additional role of inducing the action of unitary transformations on the underlying Hilbert space.

That this action preserves the algebraic properties of functionals of the type \( G_{\tilde{f}} \) can be seen by computing the Poisson bracket

\[ \{ G_{\tilde{f}}, G_{\tilde{g}} \} = \text{Tr} \sum_r \epsilon_r \left( \frac{\delta G_{\tilde{f}}}{\delta q_r} \frac{\delta G_{\tilde{g}}}{\delta p_r} - \frac{\delta G_{\tilde{g}}}{\delta q_r} \frac{\delta G_{\tilde{f}}}{\delta p_r} \right). \]  

(3.5)

We use the result that

\[ \delta G_{\tilde{f}} = \text{Tr} \tilde{f} \delta \tilde{C} \]

\[ = \text{Tr} \sum_r \{ \epsilon_r (\tilde{f} q_r - q_r \tilde{f}) \delta p_r - (\tilde{f} p_r - p_r \tilde{f}) \delta q_r \} \]

(3.6)

to obtain

\[ \frac{\delta G_{\tilde{f}}}{\delta q_r} = -[\tilde{f}, p_r], \]

(3.7)

\[ \frac{\delta G_{\tilde{f}}}{\delta p_r} = \epsilon_r [\tilde{f}, q_r], \]

and hence, expanding out the commutators, one finds that

\[ \{ G_{\tilde{f}}, G_{\tilde{g}} \} = -\text{Tr} \sum_r [\tilde{f}, \tilde{g}] (p_r q_r - \epsilon_r q_r p_r) \]

(3.8)

\[ = \text{Tr} [\tilde{f}, \tilde{g}] \tilde{C} \]

\[ = G_{[\tilde{f}, \tilde{g}]} . \]

These relations, corresponding to the group properties of integrated charges in quantum field theory, can be generalized to a “local” algebra. Defining

\[ G_{\tilde{f}_r} = \text{Tr} \tilde{f} \tilde{C}_r, \]  

(3.9)

where

\[ \tilde{C}_r = \epsilon_r q_r p_r - p_r q_r, \]  

(3.10)
one obtains in the same way that
\[ \{ \mathbf{G}_{\tilde{f}_r}, \mathbf{G}_{\tilde{g}_s} \} = \delta_{rs} \mathbf{G}_{[\tilde{f}, \tilde{g}]} r. \]  

In studying the flows induced by conserved operators, we shall also need the properties of generators projected from \( \hat{C} \). We therefore define
\[ \hat{\mathbf{G}} \tilde{f} = \text{Tr} \tilde{f} \hat{C}. \]  

Substituting (3.2), we find that the operator derivatives of \( \hat{\mathbf{G}} \tilde{f} \) with respect to the phase space variables are
\[ \frac{\delta}{\delta q_r} \hat{\mathbf{G}} \tilde{f} = (-1)^F (-1)^F \tilde{f} p_r = - \tilde{f} p_r - \epsilon_r \tilde{f}, \]  
\[ \frac{\delta}{\delta p_r} \hat{\mathbf{G}} \tilde{f} = (-1)^F (-1)^F \tilde{f} q_r = \tilde{f} q_r - \epsilon_r \tilde{f}. \]  

Computing Poisson brackets in the same way as above, we find that the algebra of the generators \( \mathbf{G}_{\tilde{f}} \) and \( \hat{\mathbf{G}} \tilde{f} \) closes,
\[ \{ \hat{\mathbf{G}} \tilde{f}, \hat{\mathbf{G}} \tilde{g} \} = \mathbf{G}_{[\tilde{f}, \tilde{g}]}, \]  
\[ \{ \hat{\mathbf{G}} \tilde{f}, \mathbf{G}_{\tilde{g}} \} = \{ \mathbf{G}_{\tilde{f}}, \hat{\mathbf{G}} \tilde{g} \} = \mathbf{G}_{[\tilde{f}, \tilde{g}]} \]  

(3.14)

which obey the algebra
\[ \{ \mathbf{G}_{\pm \tilde{f}}, \mathbf{G}_{\pm \tilde{g}} \} = \mathbf{G}_{\pm [\tilde{f}, \tilde{g}]}, \]  
\[ \{ \mathbf{G}_{+ \tilde{f}}, \mathbf{G}_{- \tilde{g}} \} = 0. \]  

(3.16)

Defining a “local” version of \( \hat{\mathbf{G}} \tilde{f} \) by
\[ \hat{\mathbf{G}}_{\tilde{f}_r} = \text{Tr} \tilde{f} \hat{\mathbf{C}}_r, \]  

(3.17)

where
\[ \hat{\mathbf{C}}_r = q_r p_r - p_r q_r, \]  

(3.18)

the algebras of (3.14) and (3.16) can be converted to local versions analogous to (3.11).

We now turn to the flows associated with \( \mathbf{G}_{\tilde{f}} \) and \( \hat{\mathbf{G}} \tilde{f} \) when used as canonical generators. Beginning with \( \mathbf{G}_{\tilde{f}} \), we consider its action on the functional \( x_s(\eta) \) defined in (2.9a),
for which $\delta x_s(\eta) = \text{Tr} \eta \delta x_s$. Defining a parameter $\gamma$ along the motion generated by $G_{\tilde{f}}$, we choose $\delta x_s$ as $dx_s/d\gamma$, so that by (2.10a) we have

$$dx_s(\eta) = \{x_s(\eta), G_{\tilde{f}}\} d\gamma. \quad (3.19)$$

Comparing (2.10b) with (3.5) and (3.19) gives

$$\frac{dq_s}{d\gamma} = [\tilde{f}, q_s], \quad \frac{dp_s}{d\gamma} = [\tilde{f}, p_s]. \quad (3.20)$$

In both the boson and fermion sectors we see that, as a solution of the differential equations (3.20), $G_{\tilde{f}}$ induces the action of a unitary group generated by $\tilde{f}$,

$$x_s(\gamma) = e^{i \tilde{f} \gamma} x_s(0) e^{-i \tilde{f} \gamma}. \quad (3.21)$$

The transformation (3.21) is unitary and norm preserving.

We next consider the canonical transformation induced on $x_s(\eta)$ by the functional $\hat{G}_{\tilde{f}}$ defined in (3.12). Introducing a parameter $\hat{\gamma}$ along the motion generated by $\hat{G}_{\tilde{f}}$, we have in this case by (2.10a),

$$dx_s(\eta) = \{x_s(\eta), \hat{G}_{\tilde{f}}\} d\hat{\gamma}. \quad (3.22)$$

Comparing (2.10b) with (3.13) and (3.22) gives

$$\frac{dq_s}{d\hat{\gamma}} = \epsilon_s (-1)^F [(-1)^F \tilde{f}, q_s] = \epsilon_s \tilde{f} q_s - q_s \tilde{f},$$
$$\frac{dp_s}{d\hat{\gamma}} = (-1)^F [(-1)^F \tilde{f}, p_s] = \tilde{f} p_s - \epsilon_s p_s \tilde{f}. \quad (3.23)$$

For the bosonic sector, (3.23) can be rewritten as

$$\frac{dq_s}{d\hat{\gamma}} = [\tilde{f}, q_s], \quad \frac{dp_s}{d\hat{\gamma}} = [\tilde{f}, p_s], \quad (3.24)$$

and can be integrated as a unitary transformation for both $q_s$ and $p_s$,

$$x_s(\hat{\gamma}) = e^{i \tilde{f} \hat{\gamma}} x_s(0) e^{-i \tilde{f} \hat{\gamma}}. \quad (3.25)$$

For the fermionic sector, however, the grading index $(-1)^F$ anticommutes with $q_s$ and $p_s$ and $\epsilon_s = -1$; consequently, the differential equations (3.23) in this case take the form

$$\frac{dq_s}{d\hat{\gamma}} = -[\tilde{f}, q_s], \quad \frac{dp_s}{d\hat{\gamma}} = \{\tilde{f}, p_s\}. \quad (3.26)$$
and involve *anticommutators* with the operator $\hat{f}$, i.e., a graded action. We note, however, that the total trace Lagrangians for which $\hat{\mathcal{C}}$ is conserved are ones in which the fermion fields appear as bosonic bilinears of the form $p_r q_s$; for these bilinears, and for the reverse ordered bosonic bilinears $q_s p_r$, we find from (3.26) that

$$\frac{d(p_r q_s)}{d\hat{\gamma}} = [\hat{f}, p_r q_s],$$
$$\frac{d(q_s p_r)}{d\hat{\gamma}} = -[\hat{f}, q_s p_r].$$

(3.27)

The solution of these differential equations is the unitary group action

$$(p_r q_s)(\hat{\gamma}) = e^{\hat{f} \hat{\gamma}}(p_r q_s)(0) e^{-\hat{f} \hat{\gamma}},$$
$$\frac{d(p_r q_s)}{d\hat{\gamma}} = [\hat{f}, p_r q_s],$$

(3.28)

which preserves the supremum operator norm of the bilinears $p_r q_s$ and $q_s p_r$. However, it is easy to see that for fermionic operators, the supremum operator norm of is not preserved by the evolution of (3.26).

Finally, it is also useful to define parameters $\gamma_\pm$ along the flows generated by $G_{\pm \hat{f}}$ according to

$$dx_s(\eta) = \{x_s(\eta), G_{\pm \hat{f}}\} d\gamma_\pm,$$

(3.29)

so that

$$\frac{dx_s}{d\gamma_\pm} = \frac{1}{2} \left( \frac{dx_s}{d\gamma_+} \pm \frac{dx_s}{d\gamma_-} \right).$$

(3.30)

Then taking sums and differences of (3.20) and (3.24), (3.26) we find that for bosons (with $x_s$ either $q_s$ or $p_s$),

$$\frac{dx_s}{d\gamma_+} = [\hat{f}, x_s],$$
$$\frac{dx_s}{d\gamma_-} = 0,$$

(3.31)

which integrate to

$$x_s(\gamma_+) = e^{\hat{f} \gamma} x_s(0) e^{-\hat{f} \gamma},$$
$$x_s(\gamma_-) = x_s(0).$$

(3.32)

Similarly, for fermions we find that

$$\frac{dq_s}{d\gamma_+} = -q_s \hat{f}, \quad \frac{dp_s}{d\gamma_+} = \hat{f} p_s,$$
$$\frac{dq_s}{d\gamma_-} = \hat{f} q_s, \quad \frac{dp_s}{d\gamma_-} = -p_s \hat{f},$$

(3.33)

which integrate to

$$q_s(\gamma_+) = q_s(0) e^{-\hat{f} \gamma_+}, \quad p_s(\gamma_+) = e^{\hat{f} \gamma_+} p_s(0),$$
$$q_s(\gamma_-) = e^{\hat{f} \gamma_-} q_s(0), \quad p_s(\gamma_-) = p_s(0) e^{-\hat{f} \gamma_-}.$$
This identifies $G_{\pm \hat{f}}$ as the generators of the one-sided unitary transformations acting on the fermions which are discussed in refs. 2 and 3.

4. The microcanonical and canonical ensembles.

Introducing a complete set of states $\{ |n\rangle \}$ in the underlying Hilbert space, the phase space operators are completely characterized by their matrix elements $\langle m | x_r | n \rangle \equiv (x_r)_{mn}$, which have the form

$$(x_r)_{mn} = \sum_A (x_r)^A_{mn} e_A, \quad (4.1)$$

where $A$ takes the values 0, 1 for complex Hilbert space, 0, 1, 2, 3 for quaternion Hilbert space (technically, a Hilbert module), and just the one value 0 for real Hilbert space, and the $e_A$ are the associated hypercomplex units (unity, complex, or quaternionic units$^2$). We restrict ourselves here to these three cases. The phase space measure is then defined as

$$d\mu = \prod_{r,m,n,A} d(x_r)^A_{mn}, \quad (4.2)$$

where redundant factors are omitted according to adjointness conditions. The measure defined in this way is invariant under canonical transformations induced by the generalized Poisson bracket.$^1$

We then define the microcanonical ensemble in terms of the set of states in the underlying Hilbert space which satisfy $\delta$-function constraints on the values of the two total trace functionals $H$, $\hat{H}$ and the matrix elements of the two conserved operator quantities $\tilde{C}$, $\hat{\tilde{C}}$ discussed in Section 1. The volume of the corresponding submanifold in phase space is given by [see ref. 11 for a somewhat more detailed discussion]

$$\Gamma(E, \hat{E}, \tilde{\nu}, \hat{\tilde{\nu}}) = \int d\mu \delta(E - H) \delta(\hat{E} - \hat{H}) \prod_{n \leq m, A} \delta(\nu^A_{nm} - \langle n \rangle (-1)^F \tilde{C} | m \rangle^A) \delta(\hat{\nu}^A_{nm} - \langle n \tilde{C} | m \rangle^A), \quad (4.3)$$

where we have used the abbreviations $\tilde{\nu} \equiv \{ \nu^A_{nm} \}$ and $\hat{\tilde{\nu}} \equiv \{ \hat{\nu}^A_{nm} \}$ for the parameters in the arguments on the left hand side. The factor $(-1)^F$ in the term with $\tilde{C}$ is not essential, but convenient in obtaining the precise form given in ref. 1 for the canonical distribution. The entropy associated with this ensemble is given by

$$S_{mic}(E, \hat{E}, \tilde{\nu}, \hat{\tilde{\nu}}) = \log \Gamma(E, \hat{E}, \tilde{\nu}, \hat{\tilde{\nu}}). \quad (4.4)$$

The operators $\tilde{C}$ and $\hat{\tilde{C}}$ are defined in terms of sums over degrees of freedom. In the context of the application to quantum field theory, the enumeration of degrees of freedom includes continuous parameters, corresponding to the measure space of the fields. These operators may therefore be decomposed into parts within a certain (large) region of the measure space, which we denote as $b$, corresponding to what we shall consider as a bath, in the sense of statistical mechanics, and within another (small) part of the measure
space, which we denote as $s$, corresponding to what we shall consider as a subsystem. We shall assume that the functionals $H$ and $\hat{H}$ may also be decomposed additively into parts associated with $b$ and $s$; this assumption is equivalent to the presence of interactions in the Hamiltonian or Lagrangian operators which are reasonably localized in the measure space of the fields (the difference in structure between the Lagrangian and Hamiltonian consists of operators that are explicitly additive), so that the errors in assuming additivity are of the nature of “surface terms”. The constraint parameters may then be considered to be approximately additive as well, and we may rewrite the microcanonical ensemble as

$$\Gamma(E, \hat{E}, \hat{\nu}, \hat{\nu}) = \int dE_s d\hat{E}_s (d\nu^s)(d\hat{\nu}^s) \Gamma_b(E - E_s, \hat{E} - \hat{E}_s, \hat{\nu} - \hat{\nu}_s, \hat{\nu} - \hat{\nu}_s) \Gamma_s(E_s, \hat{E}_s, \nu_s, \hat{\nu}_s).$$

(4.5)

We now assume that the integrand in (4.5) has a maximum which dominates the integral when there is a large number of degrees of freedom. Let us, for brevity, define (we suppress the index $s$ in the following)

$$\xi = \{\xi_i\} \equiv \{E, \hat{E}, \nu, \hat{\nu}\},$$

(4.6)

where the index $i$ refers to the elements of the set of variables, so that (4.5) takes the form

$$\Gamma(\Xi) = \int d\xi \Gamma_b(\Xi - \xi) \Gamma_s(\xi),$$

(4.7)

where $\Xi$ corresponds to the set of total properties for the whole ensemble. A necessary condition for an extremum in all of the variables at $\xi = \bar{\xi}$ is then (for every $i$)

$$\frac{\partial}{\partial \xi_i}[\Gamma_b(\Xi - \xi) \Gamma_s(\xi)]|_{\bar{\xi}} = 0,$$

(4.8)

which implies that

$$\frac{1}{\Gamma_s(\xi)} \frac{\partial \Gamma_s(\xi)}{\partial \xi_i} |_{\bar{\xi}} = \frac{1}{\Gamma_b(\Xi - \xi)} \frac{\partial \Gamma_b(\Xi - \xi)}{\partial \xi_i} |_{\bar{\xi}}.$$  

(4.9)

The logarithmic derivatives in (4.9) define a set of quantities analogous to the (reciprocal) temperature of the usual statistical mechanics, i.e., equilibrium-fixing Lagrange parameters common to the bath and the subsystem. We write these separately as

$$\tau = \frac{\partial}{\partial E} \log \Gamma_s(\xi)|_{\bar{\xi}}$$

$$\hat{\tau} = \frac{\partial}{\partial \hat{E}} \log \Gamma_s(\xi)|_{\bar{\xi}}$$

$$\lambda_{nm}^A = -\frac{\partial}{\partial \nu_{nm}^A} \log \Gamma_s(\xi)|_{\bar{\xi}}$$

$$\hat{\lambda}_{nm}^A = -\frac{\partial}{\partial \hat{\nu}_{nm}^A} \log \Gamma_s(\xi)|_{\bar{\xi}}.$$ 

(4.10)
According to the definition of entropy (4.4), the bath phase space volume is given by

\[ \Gamma_b(\Xi - \xi_s) = e^{S_b(\Xi - \xi_s)} \]

\[
\cong e^{S_b(\Xi)} \exp\{-\sum_i \xi_{i,s} \frac{\partial S_b}{\partial \xi_i}(\Xi)\}, \tag{4.11}
\]

Neglecting the small shift in argument \( \Xi \to \Xi - \xi_s \), it follows from (4.7) - (4.10) that

\[ \Gamma_b(\Xi - \xi_s) \cong e^{S_b(\Xi)} \exp\{-\tau E - \hat{\tau} \hat{E} + \sum_{n \leq m, A} (\nu_{nm}^{A}\lambda_{nm}^{A} + \hat{\nu}_{nm}^{A}\hat{\lambda}_{nm}^{A})\}. \tag{4.12} \]

We now return to (4.5), replacing the phase space volume of the bath, \( \Gamma_b \), by the approximate form (4.12), and the subsystem phase space volume \( \Gamma_s \) by the phase space integral over the constraint \( \delta \)-functions. Carrying out the integrals over the parameters, the \( \delta \)-functions imply the replacement of the parameters \( E, \hat{E}, \nu_{nm}^{A}, \hat{\nu}_{nm}^{A} \) in the exponent by the corresponding phase space quantities. Using the anti-self-adjoint properties of \( \tilde{C} \) and \( \hat{\tilde{C}} \), and defining the operator \( \tilde{\lambda} \) for which the matrix elements are \( \langle n|\tilde{\lambda}|m \rangle = \frac{1}{2}\lambda_{nm}, \quad n \neq m, \) and \( \langle n|\hat{\tilde{\lambda}}|n \rangle = \lambda_{nn} \), we see that the first term in the sum in the exponent in (4.12) is \(-\text{Tr} \tilde{\lambda} \tilde{C}\). A similar result holds for the last term of the sum (in this case, since we did not insert the factor \((-1)^F\), we obtain the \( \hat{\text{Tr}} \) functional). The volume in phase space is then

\[ \Gamma(\Xi) = e^{S_b(\Xi)} \int d\mu_s \exp\{-\tau H_s + \hat{\tau} \hat{H}_s + \text{Tr} \tilde{\lambda} \tilde{C}_s + \hat{\text{Tr}} \hat{\tilde{\lambda}} \hat{\tilde{C}}_s\}, \tag{4.13} \]

so that the normalized canonical distribution function is given by

\[ \rho = Z^{-1} \exp\{-\tau H + \hat{\tau} \hat{H} + \text{Tr} \tilde{\lambda} \tilde{C} + \hat{\text{Tr}} \hat{\tilde{\lambda}} \hat{\tilde{C}}\}, \tag{4.14} \]

where

\[ Z = \int d\mu \exp\{-\tau H + \hat{\tau} \hat{H} + \text{Tr} \tilde{\lambda} \tilde{C} + \hat{\text{Tr}} \hat{\tilde{\lambda}} \hat{\tilde{C}}\}. \tag{4.15} \]

This formula coincides with that obtained by Adler and Millard.\(^{1}\) Note that the operators \( \tilde{\lambda} \) and \( \hat{\tilde{\lambda}} \) appear as an infinite set of inverse “temperatures”, i.e., equilibrium Lagrange parameters associated both with the bath and the subsystem, corresponding to the conserved matrix elements of \((-1)^F\tilde{C}\) and \(\hat{\tilde{C}}\).

If \( \hat{\tilde{\lambda}} \) is a function of \( \tilde{\lambda} \), then the ensemble average of an operator \( \mathcal{O} \), which we denote as \( \langle \mathcal{O} \rangle_{AV} \), is a function of \( \tilde{\lambda} \) (and other scalar parameters), and hence commutes with it. If we diagonalize \( \langle \tilde{C} \rangle_{AV} \) to the form \( i_{eff} D \), and assume that \( D \) is totally degenerate\(^1\), and equal to \( \hbar \), then the analog of the equipartition (Ward) identities gives\(^1\)

\[ 0 = \langle \hbar(\dot{x}_r)_{eff} - i_{eff}[H_{eff},(x_r)_{eff}] \rangle_{AV}, \]
where we write the subscript \( \text{eff} \) to indicate the part of the operator that commutes with \( \imath_{\text{eff}} \). All of the complex canonical structure is then reproduced in the ensemble average. A second set of Ward identities\(^1\) implies that for fermionic \( q_r, p_r \),

\[
\langle \tilde{H}_{\text{eff}} q_r \rangle_{\text{AV}} = \langle p_r \tilde{H}_{\text{eff}} \rangle_{\text{AV}} = 0;
\]

from this, one sees that \( \langle \rangle_{\text{AV}} \) appears to have properties of the Wightmann vacuum.

We finally remark that the microcanonical entropy defined in (4.4) provides the Jacobian of the transformation from the integration over the measure of \( S \) in (3.15) to an integral over the parameters defining the microcanonical shells. To see this, we rewrite (4.15) as

\[
Z = \int d\mu dE d\tilde{E} (d\nu)(d\hat{\nu}) \delta(E - H) \delta(\hat{E} - \hat{H})
\]

\[
\times \prod_{n \leq m, A} \delta(\nu^A_{nm} - \langle n\rangle(-1)^F \tilde{C}|m|^A) \delta(\hat{\nu}^A_{nm} - \langle n\rangle\hat{C}|m|^A)
\]

\[
\times \exp\{-\tau E + \hat{\tau} \hat{E} + \text{Tr} \tilde{\lambda} \hat{\nu} + \text{Tr} \hat{\lambda} \tilde{\nu}\},
\]

where we have defined the anti-self-adjoint parametric operators \( \nu \) and \( \hat{\nu} \) by

\[
\nu^A_{nm} = \langle n\rangle(-1)^F \nu|m|^A, \quad \hat{\nu}^A_{nm} = \langle n\rangle\hat{\nu}|m|^A.
\]

The phase space integration over the \( \delta \)-function factors reproduces the volume of the microcanonical shell associated with these parameters, i.e., the exponential of the microcanonical entropy, so that the partition function can be written as

\[
Z = \int dE d\tilde{E} (d\nu)(d\hat{\nu}) e^{S_{\text{mic}}(E, \tilde{E}, \nu, \hat{\nu})} \exp\{-\tau E + \hat{\tau} \hat{E} + \text{Tr} \tilde{\lambda} \hat{\nu} + \text{Tr} \hat{\lambda} \tilde{\nu}\}.
\]

We now turn to study the stability of the canonical ensemble as associated with the dominant contribution to the microcanonical phase space volume. To this end, we formally define the free energy \( A \) as the negative of the logarithm of the partition function,\(^2\)

\[
Z \equiv e^{-A(\tau, \hat{\tau}, \tilde{\lambda}, \hat{\lambda})},
\]

so that (4.15) can be written as

\[
1 = \int d\mu e^{A(\tau, \hat{\tau}, \tilde{\lambda}, \hat{\lambda})} \exp\{-\tau H + \hat{\tau} \hat{H} + \text{Tr} \tilde{\lambda} \hat{C} + \text{Tr} \hat{\lambda} \tilde{C}\}.
\]

Let us now define the set of variables

\[
\{\chi_i\} = \{\tau, \hat{\tau}, -\lambda^A_{nm}, -\hat{\lambda}^A_{nm}\}.
\]

\(^2\) The conventional symbol for the free energy should not be confused with the hypercomplex index \( A \).
Differentiating (4.20) with respect to each of these, one finds (as in Eqs. (49) of ref. 1) the relations

\[ \frac{\partial A}{\partial \chi_i} = \xi_i, \]

(4.22)

where we have associated the average values of the dynamical variables \( H, \hat{H}, C_{nm}^A \) and \( C_{nm}^A \) with \( E, \hat{E}, \nu_{nm}^A \) and \( \hat{\nu}_{nm}^A \).

We now consider the identity

\[ 0 = \int d\mu (H - \langle H \rangle_{AV}) e^{A(\tau, \hat{\tau}, \tilde{\lambda}, \hat{\tilde{\lambda}})} \exp \left\{ -\tau H + \hat{\tau} \hat{H} + \text{Tr} \tilde{\lambda} \tilde{C} + \hat{\text{Tr}} \hat{\lambda} \hat{C} \right\}. \]

(4.23)

Differentiating with respect to \( \tau \), one finds

\[ 0 = \int d\mu \left( \frac{\partial A}{\partial \tau} - H \right) (H - \langle H \rangle_{AV}) e^{A(\tau, \hat{\tau}, \tilde{\lambda}, \hat{\tilde{\lambda}})} \]

\[ \times \exp \left\{ -\tau H + \hat{\tau} \hat{H} + \text{Tr} \tilde{\lambda} \tilde{C} + \hat{\text{Tr}} \hat{\lambda} \hat{C} \right\} - \frac{\partial \langle H \rangle_{AV}}{\partial \tau}, \]

(4.24)

so that, from (4.22), we find that (as in ref. 1)

\[ \langle (H - \langle H \rangle_{AV})^2 \rangle_{AV} = -\frac{\partial \langle H \rangle_{AV}}{\partial \tau} = -\frac{\partial^2 A}{\partial \tau^2} \geq 0. \]

(4.25)

In fact, applying this argument to all of the dynamical quantities (including cross terms), one can show that \( A \) is a locally convex function.11 The Taylor series expansion of \( A(\xi + \delta \xi) \), up to second order, is, with the help of the relations obtained in this way, given by

\[ A(\tau + \delta \tau, \hat{\tau} + \delta \hat{\tau}, \tilde{\lambda} + \delta \tilde{\lambda}, \hat{\tilde{\lambda}} + \delta \hat{\tilde{\lambda}}) \]

\[ = A(\tau, \hat{\tau}, \tilde{\lambda}, \hat{\tilde{\lambda}}) + \delta \tau \langle H \rangle_{AV} + \delta \hat{\tau} \langle \hat{H} \rangle_{AV} - \sum_{n \leq m, A} (\delta \lambda_{nm}^A \langle C_{nm}^A \rangle_{AV} + \delta \hat{\lambda}_{nm}^A \langle \hat{C}_{nm}^A \rangle_{AV}) \]

\[ - \frac{1}{2} \left[ \delta \tau (H - \langle H \rangle_{AV}) + \delta \hat{\tau} (\hat{H} - \langle \hat{H} \rangle_{AV}) \right] \]

\[ - \sum_{m \leq n, A} \delta \lambda_{nm}^A (C_{nm}^A - \langle C_{nm}^A \rangle_{AV}) + \delta \hat{\lambda}_{nm}^A (\hat{C}_{nm}^A - \langle \hat{C}_{nm}^A \rangle_{AV}) \]

(4.26)

the uniform negative sign of the quadratic term in the expansion indicates that \( A \) is a locally convex function, and shows that the matrix of second derivatives of \( A \) is negative semidefinite.

We now turn to the alternative expression of (4.18) for the partition function, defined in terms of an integral over the parameters of a sequence of microcanonical ensembles. The existence of a maximum in the integrand which dominates the integration assures the stability of the canonical ensemble; we show that (4.26) implies the self-consistency of our assumption of a maximum.
The conditions for a maximum of the integrand at $\xi = \bar{\xi}$ in (4.18) are that there be a stationary point, i.e., that
\[ \chi_i = \frac{\partial S_{mic}}{\partial \xi_i} |_{\bar{\xi}}, \tag{4.27} \]

**together with the requirement that the second derivative matrix**
\[ \frac{\partial^2 S_{mic}}{\partial \xi_i \partial \xi_j} = \frac{\partial \chi_i}{\partial \xi_j} \tag{4.28} \]

**should be positive definite.**

The matrix inverse to the right hand side of (4.28) is given by
\[ \frac{\partial \xi_j}{\partial \chi_i} = \frac{\partial^2 A}{\partial \chi_i \partial \chi_j}, \tag{4.29} \]

which we have shown to be a negative semidefinite matrix. This in turn implies that the matrix on the right hand side of (4.28) is negative definite, giving the condition needed to assure that the stationary point in (4.27) is indeed a (local) maximum.

Assuming this maximum dominates the integration, then the logarithm of the integral in (4.18) (up to an additive term which is relatively small for a large number of degrees of freedom) may be approximated by
\[ A \approx \tau E + \hat{\tau} \hat{E} + \text{Tr} \hat{\lambda} \hat{C} + \text{Tr} \hat{\lambda} \hat{C} - S_{mic}(E, \hat{E}, \hat{C}, \hat{C}), \tag{4.30} \]

where the arguments are at the extremal values, giving the analog of the standard thermodynamical result $A = E - TS$ for the free energy.

**Acknowledgments**

This work was supported in part by the Department of Energy under Grant #DE-FG02-90ER40542.

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