

Statistical Mechanics with Homogeneous First-Degree Lagrangians

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The equilibrium statistical mechanics is investigated of any system whose Lagrangian $L_0(v, q)$ is a convex homogeneous function of generalized velocities v , with coordinates q in a bounded set D . A member of a canonical ensemble, the system has a conjugate Hamiltonian $H_0(p, q)$ that vanishes identically in some subset $C \times D$ of its phase space. The subset C may also be specified, in some systems with a finite function $f(p, q)$, convex in $p \equiv \partial L_0 / \partial v$, and then L_0 is also convex and homogeneous in v . In either case, if C is bounded and convex, then C or the convex function f constitutes the fundamental constraint on the system. Under this fundamental constraint, it is shown that the so-called partition function becomes a phase-space volume G (classical) or a number W of micro-states (quantum) from which follows the thermodynamic fundamental relation, entropy $S \equiv k \ln G$ (or $k \ln W$).

1. INTRODUCTION

In the statistical analysis of an equilibrium thermodynamic system, the famous prescription by Gibbs is to determine the partition function Q of the system, from which follows all the thermodynamically relevant information. That is, we compute

$$\begin{aligned} Q_N &\equiv (N! h^{dN})^{-1} \int \exp(-\beta H) dp dq && \text{(classical)} \\ Q_N &\equiv \text{Trace}[\exp(-\beta H)] && \text{(quantum)} \end{aligned} \quad (1)$$

Here, $H = H_N(p, q)$ is the Hamiltonian function (classical) or operator (quantum) of the system of N particles in a d -dimensional physical space in thermal equilibrium with a heat reservoir of temperature T defined by

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$kT \equiv \beta^{-1}$, and h is Planck's constant (Feynman, 1972; Kittel, 1958). The generalized momentum of each particle is $p_i \in \mathbb{R}^d, i = 1, 2, \dots, N$; and the generalized position q_i of each particle is confined to $\Lambda \subset \mathbb{R}^d$, called the "box" of physical volume V , so that $p \equiv (p_1, p_2, \dots, p_{Nd}) \in \mathbb{R}^{Nd}$ and $q = (q_1, q_2, \dots, q_{Nd}) \in \Lambda^N \subset \mathbb{R}^{Nd}$. In the limit $N \rightarrow \infty, V \rightarrow \infty, N/V$ finite, we obtain from Q_N the free energy $F \equiv F(\beta, V, N) \equiv kT \ln Q_N$ and the internal energy $U = -\partial/\partial\beta \ln Q_N$. From F we obtain the entropy $S = S(U, V, N)$ either from the thermodynamic relation $S = (U - F)/T$ or equivalently from $S = -k \int \rho \ln \rho$, with $\rho \equiv \exp(-\beta H)/Q$, or from the Legendre transform,

$$F(\beta, V, N) \mapsto S(U, V, N) \equiv \beta \frac{\partial}{\partial \beta} \bar{F} - \bar{F}, \quad \bar{F} \equiv \beta F \quad (2)$$

in which \bar{F} is the Massieu function of S , each method involving the knowledge of Q (or equivalently of F).

In the postulatory formulation of thermodynamics, which Wightman (1979) has appropriately called neo-Gibbsian thermodynamics, perhaps best exemplified by Callen (1960), $S(U, V, N)$ is considered as the fundamental relation. That is, although Q gives F and therefore indirectly S , $F(\beta, V, N)$ is a *derived* thermodynamic potential. The question therefore arises: how do we obtain the fundamental relation $S = S(U, V, N)$ of thermodynamics directly from statistical mechanics of an open system (open with respect to energy or some other important attribute) given that statistical mechanics is the foundation of thermodynamics?

A second important question also arises: suppose we are satisfied with the indirect route of obtaining S from $F = -kT \ln Q$, what is the nature of Q if the system has a homogeneous first-degree Lagrangian $L \equiv L(\dot{q}, q)$ in $\dot{q} \equiv v$; i.e.,

$$L(\lambda v, q) = \lambda L(v, q), \quad \lambda \in \mathbb{R}_+ \quad (3)$$

where $v = \dot{q} = dq/dt$, the generalized velocity $v \in \mathbb{R}^{Nd}$ of the particles? For we know that by Euler's theorem, the Hamiltonian $H(p, q) = v \partial L / \partial v - L$ is identically zero. [Note that in many cases L is the given, from which we obtain H , to be used in equation (1), and equation (1) seems to suggest that if $H = 0$, then Q is infinite.]

In this paper we answer the second question first, and then use this to answer the first question, in cases that the Lagrangian is convex in velocity v . Of course, as noted, there is a third question: since, if $H = 0$, then $Q = \infty$, unless the domain of H is bounded, how do we obtain the thermodynamics of a system whose Hamiltonian has a bounded domain? We answer this question in cases of bounded, closed convex sets in momentum space. The

implications of the answers to the three questions are discussed in the last section of this paper.

2. PRELIMINARIES. CONVEX ANALYSIS

A function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is said to be convex (Rockafellar, 1970, especially Section 13), if for $0 \leq \theta \leq 1$, x, y in the domain of f ,

$$\text{dom } f \equiv \{x \in \mathbb{R}^n : |f(x)| < \infty\}$$

it is the case that

$$f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y) \tag{4}$$

holds. Any set $D \subset \mathbb{R}^n$ is convex if $\theta x + (1 - \theta)y \in D$ for any $x, y \in D$. We denote the closure of D by \bar{D} or C the interior of D by $\text{int}(D)$, and the boundary of D by ∂D . Also, $f(x)$ is strictly convex if for $0 < \theta < 1$, strict inequality obtains in (4).

The convex conjugate of $f(x)$ is defined by

$$f^*(x^*) = \sup\{\langle x|x^* \rangle - f(x), x \in \mathbb{R}^n\} \tag{5}$$

where $x^* \in$ dual space of \mathbb{R}^n (i.e., \mathbb{R}^n) and the scalar product of x and x^* is defined by

$$\langle x|x^* \rangle = \sum_{i=1}^n x_i x_i^* \equiv x_i x_i^* \tag{6}$$

(where repeated index denotes summation) and x^* is given by the requirement that

$$f(y) - f(x) \geq \langle y - x|x^* \rangle \quad \text{all } y \in \mathbb{R}^n \tag{7}$$

Consider a differentiable function $g: \mathbb{R}^n \rightarrow \mathbb{R}$. Its Legendre transform $g^*(x^*)$ is given by

$$g^*(x^*) \equiv \langle x|x^* \rangle - g(x) \tag{8}$$

$$x_i^* \equiv \partial g(x) / \partial x_i, \quad i = 1, 2, \dots, n$$

Rockafellar (1967) shows that if $g(x)$ is additionally strictly convex, then its Legendre transform and its convex conjugate are identical; and the transformation also effects a one-to-one mapping of $\text{int}(\text{dom } g) \rightarrow \text{int}(\text{dom } g^*)$.

We see that if $f(x)$ is convex, then

$$D \equiv \{x: f(x) < \gamma\} \subset \mathbb{R}^n, \quad \gamma \in \mathbb{R} \tag{9}$$

is an open convex set. And, as a closed convex set, $\bar{D} \equiv C$ has a support function $h(x^*)$,

$$h(x^*) \equiv \inf_{\alpha > 0} \{f^*(\alpha x^*)/\alpha + \gamma/\alpha\} \tag{10}$$

which is a homogeneous convex function generated by the convex conjugate of $f(x) - \gamma$, i.e., by $f^*(x^*) + \gamma$. The indicator function, a sort of characteristic function, of C is given by

$$\delta(x|C) \equiv \begin{cases} 0, & x \in C \\ \infty, & x \notin C \end{cases} \tag{11}$$

The domain of $h(x^*)$ is necessarily a cone, since h is homogeneous, $h(\lambda x^*) = \lambda h(x^*)$, $\lambda \in \mathbb{R}_+$, and exists for all $0 \leq \lambda < \infty$. This cone K is called the barrier cone of C , i.e.,

$$K \equiv \{x^*: \text{all } x \in C, \langle x|x^* \rangle \leq r, r \in \mathbb{R}\} \tag{12}$$

where K is a cone, means that for all $\lambda \in \mathbb{R}_+$, $x \in K \Rightarrow \lambda x \in K$. It is the case that $\delta(x|C)$ (with its domain C) and $h(x^*)$ (with its domain K) are a convex conjugate pair.

With convex conjugate transforms, we are able to handle a non-differentiable, strictly convex function f in the manner of Legendre transforms, especially functions with bounded domains, where by bounded domain we mean that

$$|x - y|^2 \equiv \langle x - y|x - y \rangle \leq R^2 < \infty$$

for all $x, y \in \text{dom } f$; [$|x| = \langle x|x \rangle^{1/2} = (x_i, x_i)^{1/2}$ is the Euclidean norm of x].

By convention, every convex function is deemed to be defined in the whole of \mathbb{R}^n , with the understanding that $f(x) = \infty$, if $x \notin \text{dom } f$. One can show easily that the intersection of a finite collection of convex sets is convex (with the empty set \emptyset taken as convex).

If $f(x)$ is homogeneous (of first order) $f(\lambda x) = \lambda f(x)$, $\lambda \in \mathbb{R}_+$, then $f(x)$ is convex if

$$f(x + y) \leq f(x) + f(y), \quad x, y \in \text{dom } f \tag{13}$$

[since $f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y) = f(\theta x) + f((1 - \theta)y)$] and strictly convex if strict inequality holds. Given a finite collection of convex functions $f_j(x), j \in J$, with respective domains C_j , it is the case that

$$f(x) \equiv \sup\{f_j(x), j \in J\} \tag{14}$$

is convex, with convex domain

$$C \equiv \bigcap_{j \in J} C_j \tag{15}$$

We may define the left scalar multiplication of convex function by $(\lambda f)(x) = \lambda f(x)$. But more relevant here is the right scalar multiplication, defined by

$$\begin{aligned} (f\lambda)(x) &= \lambda f(\lambda^{-1}x), & \lambda > 0 \\ (f0)(x) &= \delta(x|0), & f \neq 0 \end{aligned} \tag{16}$$

Then the function $g(\lambda, x)$ given by

$$g(\lambda, x) \equiv \begin{cases} (f\lambda)(x), & \lambda \geq 0 \\ \infty, & \lambda < 0 \end{cases} \tag{17}$$

is a homogeneous convex function on \mathbb{R}^{n+1} .

Finally, let us emphasize that every homogeneous convex function $h(v)$ is the support function of some closed convex set C and has a convex conjugate, defined by

$$\begin{aligned} h^*(p) &= \sup_{v \in \mathbb{R}^n} \{ \langle p|v \rangle - h(v) \} = \delta(p|C) \\ C &\equiv \{ p \in \mathbb{R}^n : \langle p|v \rangle \leq h(v), \text{ all } v \in \mathbb{R}^n \} \end{aligned} \tag{18}$$

3. SYSTEMS WITH HOMOGENEOUS LAGRANGIANS

Homogeneous Lagrangians $L_0(\dot{q}, q) \equiv L_0(v, q)$ in dynamics arise in three ways:

1. The system's Lagrangian is intrinsically homogeneous, especially in relativistic dynamics, e.g., $L_0(v, q) \equiv [G_{ij}(q)v_i v_j]^{1/2}$. We shall refer to this type as explicitly homogeneous Lagrangians. Being homogeneous, such a Lagrangian L_0 gives rise to a Legendre-transform Hamiltonian $H_0(p, q)$ which vanishes identically [by Euler's theorem $x_i \partial f / \partial x_i - kf = 0$ for $f(x)$ which is homogeneous of order $k, f(\lambda x) = \lambda^k f(x), \lambda > 0$]. More pertinent to our purpose is the fact that, being homogeneous, if also convex, L_0 is the support function of some closed convex set C given by

$$\begin{aligned} C &\equiv \{ p : \text{for all } v \in \mathbb{R}^n, p_i v_i \leq L_0(v, q) \} \\ L_0^* &\equiv \sup \{ p_i v_i - L_0(v, q), v \in \mathbb{R}^n \} \equiv \delta(p|C) \end{aligned} \tag{19}$$

and it is in this set C that the convex conjugate Hamiltonian $L_0^* \equiv H_0$ vanishes. In other words, $H_0(p, q) \equiv \delta(p|C)$, the indicator function of C . The domain of $L_0(v, q)$ is K , the barrier cone of C . In general, C can be described in terms of a set of convex functions $f_j(p, q), j \in J$, such that if

$$f(p, q) \equiv \sup \{ f_j(p, q), j \in J \}$$

then for some $\gamma \in \mathbb{R}, q \in D \equiv \Lambda^N$,

$$C \equiv \{ p : f(p, q) \leq \gamma \} \tag{20}$$

Physically $C \times D$ gives the region in phase space allowed the system. The existence of C as a nonempty, bounded, convex set [or equivalently, of $f(p, q)$] constitutes what we call a *fundamental constraint* on the system.

2. The second way is through the consideration of t as a coordinate q_0 and the transformation of $v_i \equiv dq_i/dt$ into $(dq_i/d\tau)/(dt/d\tau) \equiv v_i/v_0$, with $dt/d\tau \equiv v_0 > 0$. This transformation converts a given nonhomogeneous $L(v, q)$ into a homogeneous

$$L_0(v, q) \equiv v_0 L(v/v_0, q) \tag{21}$$

with $\text{dom } L_0 = \text{subset of } \mathbb{R}_+ \times \mathbb{R}^n$. By equation (16) we see that L_0 is the right scalar multiplication by v_0 of $L(v, q)$. In this way, any Lagrangian $L(v, q)$ can be made homogeneous. In this case, one easily shows that “action” I is preserved,

$$I = \int L(v, q) dt = \int v_0 L(v/v_0, q) d\tau \tag{22}$$

We shall refer to the Lagrangians obtained in this way as the second type or implicitly homogeneous Lagrangians. Such a Lagrangian always has at least the primary constraint

$$p_0 \equiv \partial L_0 / \partial v_0 \equiv -H = L - v_i \partial L / \partial v_i \tag{23}$$

We shall always consider that the given L is convex in v , and therefore $H(p, q)$ is convex in p , and L_0 is convex and homogeneous on \mathbb{R}^{n+1} and defines

$$\mathbb{R} \times C \equiv \{(p_0, p) : \text{for all } (v_0, v), v_0 p_0 + v_i p_i \leq L_0\}$$

For physical reasons v_0 and p_0 are usually bounded, $0 < v_0 < \infty, 0 > p_0 > -\gamma, \gamma \in \mathbb{R}_+$. Hence, with $q \in D \equiv \Lambda^N$,

$$f(p, q) \equiv H(p, q) \leq \gamma; \quad C \equiv \{p : H(p, q) \leq \gamma\} \tag{24}$$

constitute the *fundamental constraint* on the system.

3. The third way is by constraining the momenta of the system in some special way. For some physical reasons, we may not know the Lagrangian or the Hamiltonian, but know that the momenta satisfy

$$-\infty < f(p, q) \leq \gamma, \quad q \in D \tag{25}$$

where f is a constant of motion (Goldstein, 1950) and, as a supremum of some convex functions, is a strictly convex function of p , with $\text{dom } f \neq \emptyset$. This inequality (25) describes a closed convex set C ,

$$C \equiv \{p : f(p, q) \leq \gamma\}, \quad q \in D \tag{26}$$

The specification of f or C is the *fundamental constraint* on the system. The knowledge of f enables us to obtain the appropriate convex homogeneous support function $h(v, q)$ of C , [generated by $f(p, q)$], which we may take as the homogeneous Lagrangian $L_0(v, q)$ of the system. The corresponding convex conjugate Hamiltonian H_0 is the indicator function of C ,

$$H_0(p, q) \equiv \delta(p|C), \quad q \in D$$

As shown in the next section, in order to obtain the fundamental relation $S = S(U, V, N)$ one requires the proper fundamental constraint (i.e., C , which is nonempty, convex, and bounded), and this explains the terminology. We remark that our fundamental constraint differs from Dirac's primary constraint. Although both deal with the fact that the momenta are not mutually independent, the fundamental may be wholly physical, while the primary comes from the mathematical requirement that in open sets in which L_0 is twice-differentiable the Hessian $\partial^2 L_0 / \partial v_i \partial v_j$ is singular. It may happen that a set of given constraints redescribed as inequalities by $\phi_j(p, q) \leq \gamma_j$ constitutes a fundamental constraint $f(p, q) = \sup \phi_j(p, q)$. In particular, a finite collection of primary constraints in the form $p_i a_i^{(j)} = 0, j = 1, 2, 3, \dots, l$ (Raspini, 1986), modified to read $p_i a_i^{(j)} \leq \gamma_j$, for some $a_i^{(j)} \in \mathbb{R}$, may provide a fundamental constraint. This follows from the fact that

$$H^{(j)} \equiv \{p: p_i a_i^{(j)} - \gamma_j = 0\}; \quad HS^{(j)} \equiv \{p: p_i a_i^{(j)} - \gamma_j \leq 0\} \quad (27)$$

as hyperplanes and closed half-spaces, respectively, may give a nonempty, bounded, convex set C defined by

$$C \equiv \bigcap_{(j)} HS^{(j)}, \quad \partial C \equiv \bigcap_{(j)} H^{(j)} \quad (28)$$

as the p space allowed the system.

We remark that while $L_0(v, q)$ has the unbounded set K (the barrier cone of C) as its domain, the momenta $p_i = \partial L_0 / \partial v_i$ are bounded. This is because the derivative of a homogeneous function (of first order) is a homogeneous function of zeroth order, $p_i(\lambda v) = p_i(v), \lambda \in \mathbb{R}_+$. This behavior of $p_i(v)$ is also evident from the convexity of L_0 :

$$L_0(\omega, q) - L_0(v, q) \geq \langle \omega - v | p(v) \rangle, \quad \text{all } \omega \quad (29)$$

So, a fundamental constraint $f(p, q) \leq \gamma$ or C given restricts the allowed values of p or gives a closed domain $C \times D$ allowed to the system, a requirement that is eminently physical. In particular, if $f(p, q)$ is in fact $H(p, q)$ or $C \equiv \{p: H(p, q) \leq \gamma\}$, then the fundamental constraint is a restriction on the energy H [not $H_0 = \delta(p|C)$] of the system.

In this paper we consider only Lagrangians that are convex in v . This is because, in variational calculus, for the problem

$$\delta \int L(v, q) dt = 0$$

to have a solution, L must be necessarily convex in v , according to (Legendre) $\partial^2 L / \partial v_i \partial v_j$ is positive semidefinite, or (Weierstrass) $L(w, q) - L(v, q) \geq (w - v | p(v))$, all w (Clarke and Zeiden, 1986; Bolza, 1904), each of which is equivalent to convexity. So, our homogeneous Lagrangians are convex and each is therefore the support function of some convex set. For our purpose, every convex function is assumed to be nowhere minus infinity. Unless any confusion is likely, we often omit to write explicitly the q variable, with the understanding that $q \in D \equiv \Lambda^N \subset \mathbb{R}^{Nd}$, i.e., that the particles are in a bounded region, called the "box" in physical space.

4. THERMODYNAMIC FUNDAMENTAL RELATION

If the Lagrangian is homogeneous and therefore the Hamiltonian vanishes identically, then the so-called partition function is *not* defined in general. Under a prescription to be described, the "partition function" exists, but with a new interpretation as volume in phase space. This volume then furnishes the thermodynamic fundamental relation. In this section we consider the first two types of homogeneous Lagrangians and in the next section we analyze the third type.

4.1. Explicitly Homogeneous Lagrangians

Let

$$L_0: \mathbb{R}^n \times \Lambda^N \rightarrow \mathbb{R} \quad (n \equiv Nd) \quad (30)$$

be homogeneous in $v = (v_1, v_2, \dots, v_n) \in K$, a cone in \mathbb{R}^n . Then L_0 is singular in the int K , and, with $p_i \equiv \partial L_0 / \partial v_i$, $p \in \text{int } C$,

$$H_0(p, q) \equiv v_i p_i - L_0 = 0 \quad (31)$$

Suppose the matrix $M_{ij}(q) \equiv \partial^2 L_0 / \partial v_i \partial v_j$ has rank $n - l$ everywhere in $D \equiv \Lambda^N$; then there are l primary constraints (Raspini, 1986),

$$\phi_j(p, q) = 0, \quad j = 1, 2, \dots, l \equiv J, \quad q \in D \quad (32)$$

each of which is a surface in p space. And

$$\partial C \equiv \{p: \phi_j(p, q) = 0, j \in J\} \quad (33)$$

is also a surface of zero volume, and therefore, with $N_0 \equiv N! h^{Nd}$,

$$Q \equiv N_0^{-1} \int_{\text{all space}} \exp(-\beta H_0) dp dq = N_0^{-1} \int_{\partial C \times D} dp dq \quad (34)$$

which is zero. Therefore, the free energy $F(\beta, V, N) \equiv -kT \ln Q$ does not exist. Since the system is a member of a canonical ensemble, the logical prescription is to convert the surface ∂C into a volume by defining

$$C = \{p: \phi_j(p, q) \leq 0, j \in J, q \in D\} \tag{35}$$

provided ∂C is a closed surface. Then Q is replaced by

$$G = N_0^{-1} \int_{C \times D} dp dq \tag{36}$$

This integral G is the volume in phase space occupied by the system under the set of constraints (35). Note that G may be zero if C is empty, or infinite if C is *not* bounded. If C turns out to be a closed, convex, bounded set, then the set of primary constraints, redefined as inequalities, acts like a fundamental constraint. In the thermodynamic limit $N \rightarrow \infty$, the volume V of $\Lambda \rightarrow \infty$, but N/V finite, the thermodynamic fundamental relation of the system follows from Boltzmann's prescription for entropy S (Shannon, 1948, Appendix, Theorems 3 and 4, Jaynes, 1965):

$$S = S(\gamma, V, N) \equiv k \ln G; \quad G = G(\gamma, V, N) \tag{37}$$

where k is Boltzmann constant, and γ comes from the constraints. The logical interpretation of γ is a quantity that is proportional to the expectation value of some important attribute or some constant of motion $f(p, q)$, such as the internal energy $U \equiv \langle H(p, q) \rangle$; (this interpretation will be justified in Section 5 and we shall refer to $\langle f(p, q) \rangle$ as generalized internal energy), where $f(p, q)$ describes

$$C \equiv \{p: f(p, q) \leq \gamma\}, \quad q \in D$$

As a first example, consider

$$L_0(v, q) \equiv \max\{Uv_i/c_0, i = 1, 2, \dots, n\}, \quad U, c_0 \in \mathbb{R}_+ \tag{38}$$

It is known that this is the support function of

$$C \equiv \{p: p_i \geq 0, p_1 + p_2 + \dots + p_n = U/c_0\} \tag{39}$$

which is a convex, bounded set. $H_0 \equiv \delta(p|C)$. Consequently, the so-called partition function is really the volume in phase space

$$G \equiv N_0^{-1} \int_{C \times D} dp dq = N_0^{-1} V^N \int_C dp = N_0^{-1} V^N (U/C_0)^n \tag{40}$$

Then

$$1/T = k \partial S / \partial U = k \partial \ln G / \partial U \quad \text{or} \quad U = nkT = NdkT \tag{41}$$

Thus, the system with this L_0 behaves like a collection of highly relativistic classical particles.

As a second example consider

$$L_0 = [g_{ij}(q)v_i v_j]^{1/2}, \quad g_{ij}v_i v_j \geq 0 \tag{42}$$

where g is of rank $n - l$. Except for slight changes in notation, we may take over Raspini's (1986) analysis to show that the primary constraints are

$$\phi_j(p, q) \equiv p_i a_i^{(j)} = 0, \quad j = 1, 2, \dots, l$$

$p_i \equiv \partial L_0 / \partial v_i, a^{(j)} \in \mathbb{R}^n$, as in equation (32). These constraints describe hyperplanes and half-spaces as in equation (27). The intersection of these half-spaces is a closed, convex, unbounded set \hat{C} , so that these primary constraints do *not* constitute a fundamental constraint. Thus, the volume in phase space

$$\hat{G} = N_0^{-1} \int_{\hat{C} \times D} dp dq = \infty$$

in which case the fundamental relation $S = k \ln \hat{G}$ and hence the thermodynamics do not exist.

Suppose in the second example that the matrix g_{ij} is replaced by the Kronecker delta matrix $\rho^2(q)\delta_{ij}$, and L_0 is the multiple of the Euclidean norm $|v|$ plus a linear function,

$$L_0 \equiv \rho(q)(v_i v_i)^{1/2} + \langle b|v \rangle \tag{43}$$

where $\rho(q) \in \mathbb{R}_+$. That is, the v domain of L_0 is the closed convex cone, which happens to be \mathbb{R}^n . It is known that this L_0 is the support function of the bounded convex set

$$C \equiv \{p: \text{all } v, \langle p|v \rangle \leq L_0\} \tag{44}$$

which is a hypersphere of radius $\rho(q)$ centered at $b \in \mathbb{R}^n$, i.e.,

$$C = \{p: \langle p - b|p - b \rangle \leq \rho^2(q)\} \equiv B \tag{45}$$

And $H_0(p, q) \equiv \delta(p|C), q \in D$. Hence, we have

$$Q = N_0^{-1} \int_{\text{all space}} \exp(-\beta H_0) dp dq \rightarrow N_0^{-1} \int_{B \times D} dp dq \equiv G \tag{46}$$

Putting $\rho^2(q) = m\gamma$ (m is the particle mass) independent of q , we have the fundamental relation $S = S(\gamma, V, N)$. In Section 5, we show that γ is proportional to the generalized internal energy $U, \gamma = rU, r \in \mathbb{R}_+$. If $b = \underline{0} \in \mathbb{R}^n$, then C is a hypersphere of radius $(m\gamma)^{1/2}$ in n -dimensional p space, and

$$G = N_0^{-1} V^N (rU)^{n/2} (\pi m)^{n/2} / (n/2)! \tag{47}$$

from which we obtain the fundamental relation

$$S = S(U, V, N) \equiv k \ln G \sim \frac{1}{2}nk \ln U \tag{48}$$

We discuss this particular example further in Section 5, where we can infer that given $g^*(p) \equiv g^{ij}p_i p_j \leq \gamma$ and hence B , the L_0 of equation (42) is the Lagrangian of the system.

4.2. Implicitly Homogeneous Lagrangian

Let $L(v, q)$ (not explicit in t) be a nonhomogeneous, strictly convex Lagrangian with n degrees of freedom. The energy or Hamiltonian

$$H(p, q) = v_i \partial L / \partial v_i - L, \quad p \in \mathbb{R}^n, \quad q \in D \tag{49}$$

is strictly convex in p . The momenta $p_i = \partial L / \partial v_i$ are independent or equivalently the n -dimensional matrix $M_{ij} \equiv \partial^2 L / \partial v_i \partial v_j$ is nonsingular. If we transform L to

$$L_0(v, q) \equiv v_0 L(v / v_0, q) \tag{50}$$

with $v_0 = dt / d\tau$, $p_0 = \partial L_0 / \partial v_0$, $p_i = \partial L_0 / \partial v_i$, then the $(n + 1)$ -dimensional matrix

$$\bar{M}_{ij} \equiv \partial^2 L_0 / \partial v_i \partial v_j, \quad i, j = 0, 1, 2, \dots, n$$

is singular, of rank n , because L_0 is homogeneous. The convex conjugate Hamiltonian H_0 is given by

$$H_0(p, q) = v_0 p_0 + v_i p_i - L_0 = 0 \tag{51}$$

or

$$-v_0 p_0 = v_i p_i - L_0 = v_0 H(p, q)$$

That is,

$$H(p, q) + p_0 = 0 \tag{52}$$

is the single primary constraint. We assume $v_0 > 0$ and $H(p, q)$ is bounded. Consequently,

$$\mathbb{R} \times C \equiv \{(p_0, p): \text{for all } (v_0, v) \in \mathbb{R}_+ \times \mathbb{R}^n, v_0 p_0 + v_i p_i \leq L_0\} \tag{53}$$

is the fundamental constraint, because C is convex and bounded. The convex bounded set

$$C \times D \equiv \{(p, q): H(p, q) \leq \gamma\} \tag{54}$$

for some $\gamma \in \mathbb{R}_+$ is the part of the phase space allowed the system, and

$$H_0(p, q) = \delta(\hat{p} | \hat{C}); \quad \hat{p} \equiv (p_0, p), \quad \hat{C} \equiv \mathbb{R}_+ \times C \tag{55}$$

is the convex conjugate Hamiltonian of the system. As an illustration, consider as the fourth example

$$L(v, q) = \frac{1}{2}M_{ij}(q)v_i v_j \tag{56}$$

where M is a real, symmetric, n -dimensional matrix, positive-definite everywhere in D . We take it that $v_0 \equiv dt/d\tau$ is such that $0 < v_0 < \infty$. The corresponding homogeneous Lagrangian is

$$L_0(v, q) = \begin{cases} \frac{1}{2}M_{ij}v_i v_j / v_0, & 0 < v_0 < c_0 \\ 0 & v_i = v_0 = 0 \\ \infty & \text{otherwise} \end{cases} \tag{57}$$

also known as the right scalar multiplication $(Lv_0)(v)$ of L by v_0 , [see equation (16)]. The momentum p_0 equals $-H(p, q)$ and since v_0 is bounded, p_0 is bounded, $0 \geq p_0 \geq -\gamma$. Then the fundamental constraint is given by

$$C \equiv \{p: 0 \leq H(p, q) \leq \gamma\} \tag{58}$$

Define $(M^{-1})_{ij} \equiv M^{ij}$; since $H(p, q) \equiv \frac{1}{2}M^{ij}(q)p_i p_j$, we have

$$C \equiv \{p: \frac{1}{2}M^{ij}(q)p_i p_j = -p_0 \leq \gamma\} \tag{59}$$

Consequently,

$$G \equiv N_0^{-1} \int \delta(H + p_0) dp_0 dp dq = \int_{C \times D} dp dq N_0^{-1}$$

which can be done by transformation $H(p, q) \rightarrow \sum p_i^2 / 2m_i$,

$$G \equiv N_0^{-1} \int_{C \times D} dp dq |J|$$

where $\{m_i(q)\}$ are the eigenvalues of M , and $|J|$ is the Jacobian of the transformation $p \rightarrow P$ and equals one; $\det M = \prod_i m_i(q)$. Thus,

$$G = N_0^{-1} (2\gamma\pi)^{n/2} / (\frac{1}{2}n)! \int_D \prod_i m_i^{1/2}(q) dq \tag{60}$$

If M_{ij} is independent of q , then

$$G_0 = N_0^{-1} (2\pi\gamma)^{n/2} / (\frac{1}{2})! V^N (\det M)^{1/2} \tag{61}$$

which, with $S = k \ln G_0$, gives the entropy of an ideal gas in the limit $n/2 \rightarrow \infty$ and γ is identified with the generalized internal energy U_0 . In this special case $1/T \equiv \partial(k \ln G) / \partial U_0$ gives

$$U_0 = NdkT/2 \tag{62}$$

It might appear that the transformation $L \mapsto L_0$ is redundant, since one can obtain the thermodynamics from the partition function,

$$Q = N_0^{-1} \int_{\text{all space}} \exp[-\beta N(p, q)] dp dq \tag{63}$$

Actually, in the foregoing example, this integral is trivial if one makes the *unphysical* assumption, as we usually do in statistical mechanics, that the momentum or energy H is unbounded. If, however, H is bounded, which is physically logical, the integral can be quite tedious. We have

$$Q_0 = N_0^{-1} \int_{C \times D} \exp(-\beta \frac{1}{2} M^{ij} p_i p_j) dp dq \tag{64}$$

where

$$C = \{p: \frac{1}{2} M^{ij} p_i p_j \leq rU\}$$

which is hardly easy, even if M is independent of q . However, aside from the tediousness of the integration, the point is that the fundamental relation $S = S(U, V, N)$ is obtainable *directly* by the transformation $L \mapsto L_0$.

Note that [in equations (63), (64)] $Q > Q_0$, or

$$F_0 \equiv -kT \ln Q_0 > -kT \ln Q \equiv F \tag{65}$$

which shows that the fundamental constraint makes the system less stable thermodynamically than its unconstrained counterpart.

5. SYSTEMS DEFINED BY FUNDAMENTAL CONSTRAINTS

Suppose we have a system without a given Lagrangian, but for physical reasons it has, as a constant of motion, the fundamental constraint of the form convex $f_j(p, q) \leq \gamma_j, j \in J, q \in D$, which gives

$$f(p, q) \leq \gamma; \quad q \in D \tag{66}$$

where f is the pointwise supremum of $\{f_j\}$ and hence a strictly convex function in p , with nonempty $\text{dom } f \subset \mathbb{R}^n$. If we wish to compute the partition function Q , we must obtain the Hamiltonian. For this purpose, we define

$$C \equiv \{p: f(p, q) - \gamma \leq 0\}, \quad q \in D \tag{67}$$

which is a closed convex subset of the p space in which the fundamental constraint is satisfied. We shall consider only cases in which C is in fact bounded and so denotes the fundamental constraint also.

The convex conjugate of $f(p, q)$ is given as

$$f^*(v, q) \equiv \sup\{v_i p_i - f(p, q), p \in C, q \in D\} \tag{68}$$

or, if $f(p, q)$ is everywhere differentiable in p , its Legendre transform is

$$f^*(v, q) = v_i p_i - f(p, q); \quad v_i \equiv \partial f / \partial p_i \quad (69)$$

Then the support function of C is

$$h(v, q) = \inf_{\alpha > 0} \{ [f^*(\alpha v, q) + \gamma] / \alpha \} \quad (70)$$

where $v \in K$, the barrier cone of C . Since this is a well-defined function in v , we identify it with the Lagrangian $L_0(v, q)$ of the system. Since it is homogeneous, $L_0(v, q)$ furnishes the Hamiltonian $H_0(p, q)$, which is the indicator function of C ,

$$H_0(p, q) = \delta(p|C), \quad q \in D \quad (71)$$

The so-called partition function is now the volume G in phase space occupied by the system under the given fundamental constraint,

$$G = N_0^{-1} \int_{\text{all space}} \exp(-\beta H_0) dp dq = N_0^{-1} \int_{C \times D} dp dq \quad (72)$$

From this follows, as $N \rightarrow \infty$, the fundamental relation,

$$S = S(\gamma, V, N) = k \ln G \quad (73)$$

where γ is proportional to the expectation value of the attribute $f(p, q)$, i.e., to the generalized internal energy. Note that in the int C the Poisson bracket of f and H_0 vanishes.

If one insists on determining the partition function, one may, in the spirit of Dirac's treatment of primary constraints (Dirac, 1964), define

$$H(p, q) = H_0(p, q) + f(p, q) \quad (74)$$

so that

$$Q = N_0^{-1} \int_{\text{all space}} \exp(-\beta H) = N_0^{-1} \int_{C \times D} \exp(-\beta f) dp dq \quad (75)$$

from which one obtains

$$F(\beta, V, N) = -\ln Q / \beta \quad (76)$$

However, $f(p, q)$ must denote some attribute as important as energy $H(p, q)$, and therefore must be a constant of motion in order to justify equations (74)-(76).

The correctness of this approach to the thermodynamics of this system stands, whether or not L_0 or $H_0(p, q)$ gives the dynamics of the system. The point is that $L_0(v, q)$ is homogeneous, $H_0 = \delta(p|C)$, and, most important, our knowledge of C is sufficient to obtain the fundamental relation

and hence the thermodynamics of the system, if it exists, i.e., if C is nonempty, convex, and bounded. If $f(p, q)$ happens to be $H(p, q)$, then our further analysis is the same as in Section 4.2.

As a fifth example, as in Section (4.1), let

$$0 \leq f(p, q) \equiv g^{ij} p_i p_j \leq \gamma, \quad \gamma \in \mathbb{R}_+ \tag{77}$$

so that

$$C \equiv \{p: f(p, q) - \gamma \leq 0\}, \quad \text{all } q \in D \tag{78}$$

With $v_i = \partial f / \partial p_i$, the convex conjugate of $f - \gamma$ is

$$f^*(v, q) = p_i \partial f / \partial p_i - f(p, q) = g_{ij} v_i v_j + \gamma \tag{79}$$

Therefore, C has the homogeneous convex support function

$$h(v, q) = \inf_{\alpha > 0} f^*(\alpha v, q) / \alpha \tag{80}$$

By setting $d/d\alpha [f^*(\alpha v, q) / \alpha] = 0$, we have

$$h(v, q) = 2(\gamma g_{ij} v_i v_j)^{1/2} \equiv L_0(v, q) \tag{81}$$

with $g_{ij} v_i v_j \geq 0$, as the Lagrangian, under the fundamental constraint [as in equation (42)], and

$$H_0(p, q) = \delta(p|C), \quad q \in D \tag{82}$$

It is the case that C is convex and bounded, and we obtain volume G [as in equation (47)] and hence the thermodynamics of the system.

By equation (81), γ has the same dimensions as $g_{ij} v_i v_j$ and by equation (77) the same dimensions as f . Since in mechanics a Lagrangian has the dimension of energy and $g_{ij} v_i v_j$ also does, we see that γ has the dimension of energy (the energy due to the degrees of freedom pertinent to the function f). Consequently, we take γ as proportional to the generalized internal energy U , the expectation value of $f(p, q)$, of the system. We see also that one can thereby justify equation (74). We emphasize that $f(p, q)$ or U is *not* necessarily the *total* energy of the system, but the part specified by the n degrees of freedom under consideration. Of course, f may be implicitly specified by C as in section 4.1 or 4.2 or explicitly given as in this section.

6. DYNAMICS AND QUANTUM SYSTEMS

The transition to the quantum level is conceptually not different from the usual classical-to-quantum transition by the canonical quantization method, whereby $q \rightarrow \hat{q}$ and $p \rightarrow -i\hbar \partial / \partial q$ operators (Merzbacher, 1970) (or, if necessary, $p \rightarrow \hat{p}$ and $q \rightarrow i\hbar \partial / \partial p$).

The analysis of the dynamics of the first two types (explicitly and implicitly homogeneous ones) has been discussed by Dirac (1964). Here we discuss only that of the third type, in which $H_0(p, q) = \delta(p|C)$, with C defined through the fundamental constraint $-\infty < f(p, q) - \gamma \leq 0$, $q \in D$. In order to have any classical dynamics, it is necessary to define the Hamiltonian

$$H(p, q) = H_0(p, q) + f(p, q) - \gamma$$

or

$$H(p, q) = \begin{cases} f(p, q) - \gamma, & p \in C, \quad q \in D \\ \infty, & \text{otherwise} \end{cases} \quad (83)$$

From this follows the equations of dynamics,

$$v = dq/dt = \partial f/\partial p \equiv p^*; \quad dp/dt = -\partial f/\partial q \quad (84)$$

where p^* is defined as a subgradient

$$H(w, q) - H(p, q) \geq \langle w - p | p^* \rangle, \quad \text{all } w \in \mathbb{R}^n \quad (85)$$

and the particles are confined to the region $C \times D$ in phase space.

Similarly, for the quantum dynamics, we may define the operator

$$A(p, q) \equiv f(-i\hbar \partial/\partial q, q) \quad (86)$$

acting on an m -dimensional Hilbert space H . Let the eigenvectors of A be $\{\psi_j\}_1^m$, with respective eigenvalues $\{a_j\}$. Then,

$$(A - \gamma)\psi_j(q) = a_j\psi_j(q) - \gamma\psi_j(q) \quad (87)$$

and since $A - \gamma \leq 0$, we have

$$a_1 \leq a_2 \leq \dots \leq a_W \leq \gamma \quad (88)$$

where W is the number of eigenvalues of A that are no greater than γ , assuming A is self-adjoint.

Again, whether or not the above-stated dynamics is necessary, our statistical problem at the quantum level has a simple solution. Let the Hilbert space H be defined by operator A (using its eigenvectors as a basis) and let $H \equiv H_w \otimes H_B$, in which H_w is of dimension W , and Id is the identity of H_w . We have operator

$$\hat{H}_0 = \begin{cases} 0 & \text{on } H_w \\ \infty & \text{on } H_B \end{cases} \quad (89)$$

and the commutator $[A, \hat{H}_0] = 0$ on H_w . Obviously the eigenvalues of \hat{H}_0 are zeros in H_w and ∞ on H_B . Therefore, the so-called partition function

$$Q \equiv \text{Trace}[\exp(-\beta\hat{H}_0)] = \text{Tr Id} = W \quad (90)$$

which, as has been argued earlier with respect to G , is actually the number W of microstates contained in the macrostate specified by the fundamental constraint. Thus, by Boltzmann's prescription, assuming $N \rightarrow \infty$, we obtain the fundamental relation

$$S = S(\gamma, V, N) = k \ln W \tag{91}$$

where γ is proportional to the generalized internal energy $\langle A \rangle$. The thermodynamics follows under the fundamental constraint. Note that we need A and hence f to specify the Hilbert space, and the f is given explicitly as in Section 5 or implicitly through C as in Section 4.

If one insists on determining the actual partition function, one must make the argument leading to equation (84) quite logical. Assuming this has been done, or in fact that $f(p, q)$ is the energy or Hamiltonian $H(p, q)$, then, with $e_1 \leq e_2 \leq \dots \leq e_w \equiv \gamma$ one obtains

$$Q = \sum_{j=1}^w \exp(-\beta e_j) \tag{92}$$

where $\hat{H}\psi_j = e_j\psi_j$ and obviously W and hence Q depend on V, N and $\gamma \equiv rU, r \in \mathbb{R}_+, U \equiv \langle \hat{H} \rangle$. Thus,

$$-\ln Q/\beta \equiv F = F(\beta, V, N)$$

We envisage that it must be a difficult task to compute such Q in general, whereas computing $G \equiv W$ requires *counting* those e 's that are less than or equal to γ and using combinatorics.

Let us take as a sixth example an ideal gas of N bosons in a cubic "box" of side L , or $\Lambda \equiv \{q: 0 \leq q_i \leq L\}$, and under the fundamental constraint

$$0 < f(p, q) = \alpha \langle p|p \rangle \leq \gamma \Rightarrow |p| \leq (\gamma/\alpha)^{1/2} \tag{93}$$

The operator

$$A(p, q) = - \sum_{i=1}^n \alpha \hbar^2 d^2/dq_i^2$$

gives

$$-\alpha \hbar^2 \frac{d^2}{dq_i^2} \psi_j(q) = a_j \psi_j(q), \quad 0 \leq q_i \leq L \tag{94}$$

so that

$$\psi_j(q) = b_j \sin(p_j q / \hbar); \quad p_j = j\pi\hbar/L \tag{95}$$

Using the constraint, we have

$$j \leq (L/\pi\hbar)(\gamma/\alpha)^{1/2} = (L/\pi\hbar)(rU/\alpha)^{1/2} \equiv J \tag{96}$$

That is, the number of microstates is $W = (N + J)!/N!J!$; and

$$S = 3k \ln W \Rightarrow 1/kT = 3N/(2\lambda U^{1/2}) \ln(1 + \lambda/U^{1/2})$$

where $\lambda = N\pi\hbar(\alpha/r)^{1/2}/L$; for high U , $U = 3NkT/2$.

We also have, with $C = \{p: |p| \leq (\gamma/\alpha)^{1/2}\}$,

$$L_0(v, q) = (2\gamma\alpha)^{1/2}|v|, \quad H_0 = \delta(p|C), \quad q \in D$$

and also

$$H(p, q) = -\sum_1^n \alpha \hbar^2 d^2/dq_i^2, \quad q \in D \quad (97)$$

each of which has the eigenvalues

$$e_j = (\alpha\pi^2\hbar^2/4L^2)j^2; \quad j = 1, 2, \dots, (2L/\pi\hbar)(\gamma/\alpha)^{1/2} \equiv J \quad (98)$$

Then,

$$Q = Q_1^n; \quad Q_1 = \sum_{j=1}^J \exp(-\beta\alpha\pi^2\hbar^2j^2/L^2) \quad (99)$$

One may compare the tasks involved in obtaining S from equation (96) and obtaining S or F from equation (99).

7. DISCUSSION

Given a system that is a member of a canonical ensemble, if its Lagrangian is homogeneous (of first degree), we obtain the volume G in phase space allowed the system, instead of the usual partition function Q . Analytically speaking, since every convex homogeneous function is the support function of some convex set defined by a convex function, it follows that a system with a homogeneous Lagrangian is a system obeying some constraint of the type

$$\begin{aligned} -\infty < f(p, q) \leq \gamma, \quad p \in C, \quad q \in \Lambda^N \\ C \equiv \{p: f(p, q) \leq \gamma = rU\} \end{aligned} \quad (100)$$

called a fundamental constraint. If f is convex or C is convex and bounded, then computing G under this constraint provides the fundamental relation entropy $S = S(U, V, N) = k \ln G$ and hence the thermodynamics of the system. Usually, $f(p, q)$ is an attribute or a constant of motion (such as the Hamiltonian) of the system.

A system may have an explicitly homogeneous Lagrangian (as in relativistic systems), an implicitly homogeneous Lagrangian (in an attempt to avoid a privileged observer), or an imposed homogeneous Lagrangian, imposed by physical considerations. For each case, one winds up with a

fundamental constraint, whether or not the necessary convex function $f(p, q)$ is explicitly or implicitly given. The fundamental constraint is in general a recognition of the fact that the momenta are not a set of independent variables, or that their domain is nonempty and bounded, whereas those of the velocities are unbounded.

At the quantum level, it is also a well-defined program to determine the number W of microstates that are consistent with the macrostate specified by the fundamental constraint. Here, it is assumed that $f(p, q)$ has been turned into an operator $A(p, q)$ on a suitable Hilbert space, and that the operator A has suitable properties such as self-adjointness.

Finally, if a system with homogeneous Lagrangian has no proper fundamental constraint [$f(p, q)$ is proper if it is strictly convex and $\text{dom } f$ or C is nonempty, convex, and bounded], then the system has no thermodynamics. That is, it is not in a thermal equilibrium with any heat reservoir. Of course, in some cases, one does not know $f(p, q)$; but if convex C is known, its boundedness or lack of it is sufficient to determine if the system has some thermodynamics.

Our conclusions are as follows:

(i) Given an intrinsically homogeneous Lagrangian $L_0(v, q)$, we determine *not* the partition function Q , but the volume in phase space

$$G = (N! h^{Nd})^{-1} \int_{C \times D} dp dq$$

after determining the appropriate fundamental constraint signified by the closed, bounded, convex set C if there is one. The fundamental relation $S = k \ln G$ and the thermodynamics of the system are obtained thereby, and this is the answer to our second question.

(ii) Given convex L , we transform L to homogeneous L_0 and determine G and hence the fundamental relation $S = S(U, V, N)$, as in (i). This answers our first question.

(iii) Given no L or H , but convex $f(p, q)$, some constant of motion, as the fundamental constraint explicitly expressed or implicitly expressed in terms of bounded convex C , we determine G and S as in (i). And this is the answer to our third question.

The program in (ii) may be unnecessary, but it could bear some remarkable results, especially if momenta are bounded. In (i) we have the only directly plausible method, and in (iii) the only feasible program.

Finally, we remark that in the thermodynamic limit the value of r in equation (100) is inconsequential (Shannon, 1948; Jaynes, 1965), and we may set it equal to 1. That is, according to Jaynes (1965), in the limit $N \rightarrow \infty$, our foregoing results are independent of whatever is considered to be the phase space (or microstates) of "reasonable probability."

REFERENCES

- Bolza, O. (1904). *Lectures on the Calculus of Variations*, University of Chicago Press. [Reprinted, Chelsea, New York, 1961, 1973].
- Callen, H. B. (1960). *Thermodynamics*, Wiley, New York.
- Clarke, F. H., and Zeiden, V. (1986). Sufficiency and the Jacobi condition in the calculus of variations, *Canadian Journal of Mathematics*, **38**, 1199–1209.
- Dirac, P. A. M. (1964). *Lectures in Quantum Mechanics*, Yeshiva University Press, New York.
- Feynman, R. P. (1972). *Statistical Mechanics*, Benjamin, Reading, Massachusetts.
- Goldstein, H. (1950). *Classical Mechanics*, Addison-Wesley, Reading, Massachusetts.
- Jaynes, E. T. (1965). Gibbs versus Boltzmann entropies, *American Journal of Physics*, **33**, 391–398.
- Kittel, C. (1958). *Elementary Statistical Physics*, Wiley, New York.
- Merzbacher, E. (1970). *Quantum Mechanics*, Wiley, New York.
- Raspini, A. (1986). Structure of the primary Hamiltonian constraints for a singular N -body Lagrangian, *International Journal of Theoretical Physics*, **25**, 737–739.
- Rockafellar, R. T. (1967). Conjugates and Legendre transforms of convex functions, *Canadian Journal of Mathematics*, **19**, 200–205.
- Rockafellar, R. T. (1970), *Convex Analysis*, Princeton University Press, Princeton, New Jersey.
- Shannon, C. E. (1948). A mathematical theory of communication, *Bell System Technical Journal*, **27**, 379–423.
- Wightman, A. S. (1979). Introduction to R. B. Israel, *Convexity in the Theory of Lattice Gases*, Princeton University Press, Princeton, New Jersey.