In the present paper, we illustrate a simple geometric approach to measure thermodynamic observables within the microcanonical ensemble, in systems described by a Hamiltonian $H$, and with $K \geq 0$ independent conserved quantities, we derive the microcanonical thermodynamics for this system, is given in terms of the microcanonical entropy $S(v_0)$. Among the equivalent ex-

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In spite traditionally, the microcanonical ensemble has played a minor role respect to the canonical and grand-canonical approach, in reason of the more complicated formulation of the statistical formulas, nowadays, thanks to the performance provided by the current computers, the microcanonical simulation is probably the most used tool in physics. Molecular dynamics is applied for investigations that cover the fields of the dynamics of nonlinear semi-classical systems, the living matter issues (protein folding, DNA-helix), the dynamics of nanosystems and so on. The ergodicity in fact, whenever holds true, allows to measure dynamic observables as temporal averages of appropriate functionals along the dynamical evolution, instead of perform integrals (often unmanageable) on the phase space. In this contest have been written very famous papers [1], that date back to the early applications of molecular-dynamics in physics. However, their application is restricted to systems described by a separable Hamiltonian, i.e. given by a standard term of kinetic energy plus an interaction potential term. In a series of more recent papers [2,3], Rugh has developed a microthermodynamic formalism to measure thermodynamical functions in the microcanonical ensemble. The Rugh’s formalism applies to non-separable Hamiltonian systems, and to the case of Hamiltonians that depend on parameters.

In the present paper, we illustrate a simple geometric approach to measure thermodynamic observables within the microcanonical ensemble, in systems described also by nonstandard Hamiltonians [4] and with an arbitrary number of first integrals. We consider a classical many-particle system described by a Hamiltonian $H(x^1, \ldots, x^{N+k})$ which, in addition to the total energy $H$, has $K \geq 0$ independent conserved quantities $V_j(x, x^{N+k}) = v_j$ such that $\{H, V_j\} = 0$ for $j = 1, \ldots, K$. All the first integrals are assumed to be in involution. We derive in detail the expressions for the microcanonical entropy (i.e. the expression of the microcanonical invariant measure), and we give the general formulas that allow to measure all the thermodynamic function as the temperature, the chemical potential, the specific heat, the pressure, and so on. More precisely, we show that entropy and the other thermodynamic functions are derived by multidimensional integrals performed over the sub-manifolds given by the intersection of the constant energy hyper-surfaces $H(x^1, x^{N+k}) = v_0$ with those defined by $V_j(x^1, x^{N+k}) = v_j$ for $j = 1, \ldots, K$. In particular, we show that all order derivatives of the entropy with respect to the $v_j$ for $j = 0, \ldots, K$, from which the microcanonical observables depend on, can be calculated as time averages along the time evolution of appropriate functions, whenever the hypothesis of ergodicity holds true. In order to simplify the notations, let us introduce the following definitions: with $x := (x^1, x^{N+k})$ we indicate a generic point of the system phase-space, with $V_0(x) := H(x)$ the “first” of the conserved quantities, and with $\Lambda_{v_j} = \{x \in \mathbb{R}^{N+k} | V_j(x) = v_j\}$ for $j = 0, \ldots, K$ the hyper-surface associated to the $K+1$ conserved independent quantities. We shall assume the level sets of $V_j$ to be non-singular hyper-surfaces. Even if the hyper-surfaces $\Lambda_{v_j}$, in general, constitute a singular foliation, since for some values of $v_j$ an hyper-surface is not a differential manifold, for generic values of $v_j$ this is not an issue. Furthermore, we will indicate with $V = (V_0, \ldots, V_K)$ a vector whose components are the conserved quantities, and with $v = (v_0, \ldots, v_K)$ the vector of the corresponding values, for a generic configuration. In addition, we will indicate with $M_K(v) \subset \mathbb{R}^{N+k}$ the set given by the intersection of the hyper-surfaces $\Lambda_{v_j}$, for $j = 0, \ldots, K$, that is $M_K(v) = \bigcap_{j=0}^K \Lambda_{v_j}$. We shall give the proof of statements reported above, in three steps, according to the choice $K = 0, 1$ and for an arbitrary value of $K$.

**Case $K = 0$—**Let us begin by summarizing the results of Ref. [3,4]. Let $H(x)$ be a classical Hamiltonian describing an autonomous many-body system whose coordinates and canonical momenta are represented as $N$-component vectors $x \in \mathbb{R}^{N}$. Let us suppose that this system has just one conserved quantity, that is the total energy $H$. The microcanonical description of equilibrium thermodynamics for this system, is given in terms of the microcanonical entropy $S(v_0)$. Among the equivalent ex-
pressions allowed for $S(v_0)$ one can consider the surface entropy $[4] S(v_0) = \ln \int d^N x \delta(V_0(x) - v_0)$, in [2] it is shown the following identity

$$S(v_0) = \ln \int_{\Lambda_{v_0}} m^N(V_0) \parallel \nabla V_0 \parallel .$$

This expression has a precise geometrical interpretation. In fact, $m^N(V_0) = \sum_{j=1}^N (1 - j^{-1/2}) dx_1 \cdot \ldots \cdot dx_N$ is the metric induced from $\mathbb{R}^N$ on the hyper-surface $\Lambda_{v_0}^N$, where $n^0_j = \partial V_0 / \parallel \nabla V_0 \parallel$ are the components of the unitary vector orthogonal to the hyper-surface, and $1 / \parallel \nabla V_0 \parallel$ is the microcanonical measure. The symbol $dx_j$, means that $dx_j$ has been lifted from the formula. The microcanonical thermodynamics is obtained by calculating the derivatives of $S(v_0)$. This fact allows a geometric interpretation of all thermodynamic quantity. E.g. the inverse temperature is given by the definition $1 / T(v_0) = \partial S(v_0) / \partial v_0$. This quantity can be rewritten in a geometric form by using the Federer-Laurence derivation formula [2][11]

$$\frac{\partial}{\partial v_0} \int_{\Lambda_{v_0}} m^N(V_0) \psi = \int_{\Lambda_{v_0}} m^N(V_0) A^k(V_0, \psi) \hspace{1cm} (1)$$

where, by setting $n^0 = \nabla V_0 / \parallel \nabla V_0 \parallel$, it is

$$A(V_0, \psi) = 1 / \parallel \nabla V_0 \parallel \nabla (n^0 \psi) . \hspace{1cm} (2)$$

In fact, the microcanonical temperature results (see [2] for details)

$$\frac{1}{T(v_0)} = \frac{\int_{\Lambda_{v_0}} m^N(V_0) / \parallel \nabla V_0 \parallel \nabla (n^0 / \parallel \nabla V_0 \parallel)}{\int_{\Lambda_{v_0}} m^N(V_0) / \parallel \nabla V_0 \parallel} ,$$

that is, the microcanonical average of $\nabla (n^0 / \parallel \nabla V_0 \parallel)$ on the energy hyper-surface $\Lambda_{v_0}^N$.

Case $K = 1$.—Let us consider a system described by the Hamiltonian $H(x^1, \ldots, x^{N+1})$ which has in addition to the total energy $H$, one independent conserved quantity $V_1(x^1, \ldots, x^{N+1}) = v_1$ such that $\{H, V_1\} = 0$. Consistently with the previous case, the microcanonical entropy is given by $S(v) = \ln \int d^{N+1} x \delta(V(x) - v)$, where $\delta(V(x) - v) = \prod_{j=0,1} \delta(V_j(x) - v_j)$. The second delta function has been added in order to take in account of the second first-integral of motion. In [12] it has been shown that

$$S(v) = \ln \int_{\mathcal{M}_1} \frac{m^{N+1}(V_0, V_1)}{\parallel \Pi_1 \parallel} ,$$

where $\mathcal{M}_1$ is the intersection set of the hyper-surfaces $\Lambda_{v_0}^N$ and $\Lambda_{V_1}^1$. The measure $m^{N+1}(V_0, V_1)$ is that one induced by $\mathbb{R}^{N+1}$ on $\mathcal{M}_1$, that is

$$m^{N+1}(V_0, V_1) = \sum_{(n,<,\infty)} (-1)^{n-\infty} F_{\mu,0} d\mu d\xi_1 \cdot \ldots \cdot d\xi_{\nu} \ldots d\xi_{N+1}$$

where $F_{\mu,0} = (e_\mu^0, e_{\mu,0}^0, e_{\mu,0}^1)$ depends on the unitary vectors of a basis $\{e_0^0, e_1^0\}$ are derived by the normalized gradient vectors $n_j = \nabla V_j / \parallel \nabla V_j \parallel$ for $j = 0, 1$, by means of a Gram-Schmidt orthonormalization process, starting from the vector $e^1 = n^1$. Thus, $e^0 = [n^0 - (n^0 \cdot n^1)n^1] / [1 - (n^0 \cdot n^1)]^{1/2}$. Furthermore $\Pi_1 = \nabla V_0 \wedge \nabla V_1$, where $\nabla V_j = \sum \partial \mu_j \nabla V_{\mu,0}^j$ for $j = 0, 1$. In order to derive the temperature in the microcanonical ensemble, according to the definition $T(v) = (\partial S(v_0, v_1) / \partial v_0)^{-1}$, we shall use the following generalization of the Federer-Laurence derivation formula [11][2], whose proof is given below. The generalized derivation formula results [13]

$$\frac{\partial}{\partial v_0} \int_{\mathcal{M}_1} m^{N+1}(V_0, V_1) \psi = \int_{\mathcal{M}_1} m^{N+1}(V_0, V_1) A^k(V_0, V_1, \psi) \hspace{1cm} (3)$$

where

$$A_1(V_0, V_1, \psi) = \frac{1}{\nabla V_0 \cdot e_0^0} [\nabla (e^0 \psi) - \psi e^1 \cdot (e^1 \cdot \nabla) (e^0)] , \hspace{1cm} (4)$$

is meant as a function of $V_0$ and $V_1$ also through the dependence from these latter of the unitary vectors $e^0$ and $e^1$. Here, and in the following we mean $e^1 \cdot (e^1 \cdot \nabla) (e^0) = \sum_{j,k} e_1^j e_1^k \partial \mu^k \partial v_j (e^0_j)$. By the calculation reported above, we can easily derive $\partial S(E, v_1) / \partial v_1$ that, when $V_1$ is the total number of atoms, gives the chemical potential via the definition $\mu / T = - \partial S(E, v_1) / \partial v_1$. Indeed, by exchanging $V_0$ with $V_1$ and $v_0$ with $v_1$, it is easy derive from Eq. [3] the following formula

$$\frac{\partial}{\partial v_1} \int_{\mathcal{M}_1} m^{N+1}(V_0, V_1) \psi = \int_{\mathcal{M}_1} m^{N+1}(V_0, V_1) B^k(V_0, V_1) \hspace{1cm} (5)$$

where

$$B_1(V_0, V_1, \psi) = A_1(V_1, V_0, \psi) . \hspace{1cm} (5)$$

Obviously

$$\frac{\partial}{\partial v_1} \int_{\mathcal{M}_1} m^{N+1}(V_0, V_1) \psi = \int_{\mathcal{M}_1} m^{N+1}(V_0, V_1) B^k(V_0, V_1, A^k(V_0, V_1, \psi)) . \hspace{1cm} (6)$$

Proof of the generalization of the Federer-Laurence derivation formula.—In this section we shall give the proof of the generalization of the Federer-Laurence theorem to varieties of co-dimension two. As first step we shall calculate $\partial (\int_{\mathcal{M}_1} \psi m^{N+1}(V_0, V_1)) / \partial v_0$ and, by iteration, we will achieve our aim. In this derivation we make use of the Stokes theorem. Let $U$ be a subset of $\Lambda_1^1$, such that $\partial U = \partial \mathcal{M}_1(v_0 + \Delta v_0, v) \cup \partial \mathcal{M}_1(v_0, v)$. The Stokes theorem states

$$\int_{\partial U} \omega = \int_U d \omega . \hspace{1cm} (7)$$
Let us choose $\omega = \psi^{m^{N+1}}(V_0, V_1)$, thus we obtain
\[
d \omega = \sum_{\nu = 1}^{N+1} (-1)^{\nu} \partial_\nu (\psi F_{\nu\mu}) dx_1 \ldots dx_\mu \ldots dx_{N+1}
\]
and, by using the definition of $F_{\nu\mu}$, it follows
\[
\int_U d \omega = \int_U \left[ \nabla \cdot (\psi e^0) - \psi e^1 \cdot (e^1 \cdot \nabla) (e^0) \right] m^{N+1}(V_1).
\]
Now it is easy to verify that
\[
m^{N+1}(V_1) = \sum_{\alpha} e^{0}_\alpha dx_\alpha \wedge m^{N+1}(V_0, V_1),
\]
therefore, by choosing vectors orthogonal to $\mathfrak{M}_1(v_0, v)$ and $\mathfrak{M}_1(v_0 + \Delta v_0, v)$ (but tangent to $\Lambda_v$) with opposite orientations, we get from the Stokes theorem
\[
\int_{\mathfrak{M}_1(v_0, v)} \psi m^{N+1}(V_0, V_1) - \int_{\mathfrak{M}_1(v_0, v)} \psi m^{N+1}(V_0, V_1) = \int_0^\Delta v_0 d s \int_{\mathfrak{M}_1(v_0 + s v, v)} m^{N+1}(V_0, V_1) \times
\]
\[
1 \nabla V_0 \cdot e^0 \left[ \nabla \cdot (\psi e^0) - \psi e^1 \cdot (e^1 \cdot \nabla) (e^0) \right],
\]
that, in the limit $\Delta v_0 \to 0$ gives Eq. (3) for $k = 1$, by iteration the generalization of the Laurence-Federer formula is proved.

General case. In this section we will derive the microcanonical entropy, and its derivatives with respect to the conserved quantities, in the case of systems with $K > 1$ first integrals in addition to the energy.

Let a system be described by the Hamiltonian $H(x)$ that depends on $x = (x^1, \ldots, x^{N+K})$. Let us suppose the system to have, in addition to the total energy $H$, $K$ independent conserved quantity $V_j(x) = v_j$ such that $(H, V_j) = 0$ for $j = 1, \ldots, K$. The microcanonical entropy is given by $S(v) = \ln \mathfrak{M}^{N+K} \text{d} \delta(V(x) - v)$, where $\delta(V(x) - v) = \prod_{j=0}^{K} \delta(V_j(x) - v)_j$. In this case
\[
S(v) = \ln \int_{\mathfrak{M}_K} \frac{m^{N+K}(V)}{||\Pi_K||},
\]
where $\mathfrak{M}_K$ is the intersection set of the hyper-surfaces $\Lambda_{v_0}^{j}$ for $j = 0, \ldots, K$, $V = (V_0, \ldots, V_K)$ and $v = (v_0, \ldots, v_K)$. The measure $m^{N+K}(V)$ is that one induced by $\mathbb{R}^{N+K}$ on $\mathfrak{M}_K$, and it is defined as follows.

Let $n^j = \nabla V_j / ||\nabla V_j||$ be the unitary vectors orthogonal to the hyper-surfaces $\Lambda_{v_0}^{j}$, for $j = 0, \ldots, K$. By the Gram-Schmidt orthonormalization process, starting from the set of $K + 1$ independent unitary vectors $\{n^0, \ldots, n^K\}$, we can obtain the following orthonormalized basis $\{e^0, \ldots, e^K\}$, where $e^K = n^K$. Therefore, the measure $m^{N+K}(V)$ results
\[
m^{N+K}(V) = s(e^K \wedge \cdots \wedge e^0),
\]
where $e^j = \sum_{\alpha} e^{j}_\alpha dx_\alpha$, for $j = 0, \ldots, K$, and $s$ is the (Hodge) star operator. The microcanonical measure is the norm of
\[
\Pi_K = \nabla V_0 \wedge \nabla V_1 \wedge \cdots \wedge \nabla V_K,
\]
where $\nabla V_j = \sum_{\nu} \partial_\nu V_j dx^\nu$, for $j = 0, \ldots, K$.

For convenience let us introduce the following notation: $(\overline{v}) = (v_1, \ldots, v_K)$ and $\overline{V} = (V_1, \ldots, V_K)$. Let us calculate the derivative of entropy with respect to $v_0$, the derivative with respect to the other variables are obtained easily by cyclic permutation of the indices. Also here we resort to the Stokes theorem where, in this case, $U$ is a sub-set of the intersection set of the hyper-surfaces $\Lambda_{v_0}^{j}$ for $j = 1, \ldots, K$, in such a way that $\partial U = \mathfrak{M}_K(v_0 + \Delta v_0, v) \cup \mathfrak{M}_K(v_0, v)$. Furthermore, we choose $\omega = \psi^{m^{N+K}}(V)$, thus the following facts hold true
\[
m^{N+K}(\overline{V}) = \sum_{\alpha} e^{0}_\alpha dx_\alpha \wedge m^{N+K}(V),
\]
where $m^{N+K}(\overline{V}) = s(e^K \wedge \cdots \wedge e^1)$
\[
\int_{\mathfrak{M}_K(v_0 + \Delta v_0, \overline{V})} \psi m^{N+K}(V) - \int_{\mathfrak{M}_K(v_0, \overline{V})} \psi m^{N+K}(V) \times
\]
\[
\int_0^\Delta v_0 d s \int_{\mathfrak{M}_1(v_0 + s v, \overline{V})} m^{N+K}(V) \times
\]
\[
1 \nabla V_0 \cdot e^0 \left( d \omega, s(e^K \wedge \cdots \wedge e^1) \right),
\]
where $(,)$ is the inner product. Thus we have
\[
\frac{\partial}{\partial v_0} \int_{\mathfrak{M}_K} m^{N+K}(V) \psi = \int_{\mathfrak{M}_K} m^{N+K}(V) A_K^{j}(V, \psi) \quad (9)
\]
where
\[
A_K(V, \psi) = \frac{1}{||\nabla V_0|| e^0} (d \omega, s(e^K \wedge \cdots \wedge e^1)).
\]

Application to the discrete nonlinear Schrödinger equation. With reference to the standard canonical coordinates, the Hamiltonian of the discrete nonlinear Schrödinger equation (DNSE) writes
\[
H_\alpha(p, q) = \Lambda_\alpha \sum_j \left( p_j^2 + q_j^2 \right) - \tau_\alpha \sum_j (p_j p_{j+1} + q_j q_{j+1}),
\]
where $\Lambda_\alpha$ and $\tau_\alpha$ measure the magnitude of the repulsive on-site interaction and of the hopping intensity, respectively. Here, the index $j$ numbers the sites from 1 to $M$ and periodic boundary conditions are assumed. This Hamiltonian describes the dynamics of a system of a Bose-Einstein condensate (BEC) of repulsive-atoms, in an optical lattice in the superfluid regime. The model possesses two conserved quantities: the energy $V_0 = H_\alpha$ and the number of particles $V_1 = \sum_j (q_j^2 + p_j^2) / 2$. Thus, it corresponds to the case $K = 1$ of the present paper. Under the hypothesis that the ergodicity holds true, for
this system the temperature, as a function of the total energy \(E\) and number of atoms \(N\), can be measured as a temporal average along the dynamical evolution. By using Eq. 11 we get
\[
\frac{1}{T(E,N)} = \lim_{s \to \infty} \frac{1}{s} \int_0^s ds' \langle \Phi(x(s')) \rangle,
\]
where
\[
\Phi(x) = \frac{\|\Pi_1\|}{\nabla H \cdot e^0} \left[ \nabla \left( \frac{e^0}{\|\Pi_1\|} \right) - \left( \frac{e^1}{\|\Pi_1\|} \right) \cdot e^1 \right],
\]
is written in terms of \(e^1 = \nabla V_1/\|\nabla V_1\|\) and
\[
e^0 = \left[ n^0 - (n^0 \cdot e^1) e^1 \right]/\left[ 1 - (n^0 \cdot e^1)^2 \right]^{1/2},
\]
where \(n^0 = \nabla H_\alpha/\|\nabla H_\alpha\|\). Furthermore it results
\[
\|\Pi_1\| = \left( \sum_{\mu,\nu=1}^{N+1} \frac{\partial H_\alpha}{\partial x_\mu} \frac{\partial V_1}{\partial x_\nu} - \frac{\partial H_\alpha}{\partial x_\nu} \frac{\partial V_1}{\partial x_\mu} \right)^2
\]
with and \(x_{2\mu-1} = q_\mu, x_{2\mu} = p_\mu\) are the \(M = (N+1)/2\) lattice coordinates. By exchanging \(H_\alpha\) with \(V_1\), and vice versa, in these equations we can measure the chemical potential. In Ref. 13, these formulas have been checked and used to explore the thermodynamics of the DNSE where it has been observed the existence of negative temperature states. Analogously, in Ref. 15 the microcanonical approach proposed by Rugh, has been applied in the context of Bose-Einstein condensates, studying the projected Gross-Pitaevskii equation.

Application to the BEC mixtures.—The dynamics of a mixture of two bosonic species, condensed in an optical lattice and in the superfluid regime is described by two coupled DNSEs and the Hamiltonian writes
\[
H(p,q;\tilde{p},\tilde{q}) = H_1(p,q) + H_2(\tilde{p},\tilde{q}) + \beta \sum_j (q_j^2 + p_j^2)(\tilde{p}_j^2 + \tilde{q}_j^2),
\]
where \(\beta\) takes into account the interaction between the two species, and by assuming periodic boundary conditions the index \(j\) runs from 1 to \(M\). In this case there are three conserved quantities the total energy \(V_0 = H\), and the total number of atoms of each species: \(V_1 = \sum j (q_j^2 + p_j^2)/2\) and \(V_2 = \sum j (\tilde{p}_j^2 + \tilde{q}_j^2)/2\). Thus, we have to use the formulas of the case \(K = 2\) and, from Eq. 10 the inverse temperature is measured as the microcanonical average of the function
\[
\Phi_2(x) = \frac{\|\Pi_2\|}{\nabla H \cdot e^0} \sum_{\mu<\nu} A_{\mu\sigma} \delta_{\mu\sigma} e^2_{\mu\sigma},
\]
where \(\delta\) is the Kronecker’s delta and
\[
A_{\mu\sigma} = \sum_{\rho=1}^{N+K} \sum_{i,j,k=0}^2 \varepsilon_{ijk} \left[ \partial_{\rho}(\psi) (e_{\rho}^i e_{\rho}^j e_{\rho}^k) + \psi \partial_{\rho} (e_{\rho}^i e_{\rho}^j e_{\rho}^k) \right].
\]
Here, \(\varepsilon\) is the completely antisymmetric tensor, the unitary vectors are \(e_{\rho}^j = \nabla V_j/\|\nabla V_j\|\) for \(j = 1,2\), and \(e^0 = \eta/\|\eta\|\), where
\[
\eta = n^0 - (n^0 \cdot e^1) e^1 - (n^0 \cdot e^2) e^2,
\]
and \(n^0 = \nabla H/\|\nabla H\|\). Finally, from Eq. 8 we have
\[
\|\Pi_2\| = \left( \sum_{\rho=1}^{N+K} \sum_{i,j,k=0}^2 \varepsilon_{ijk} \frac{\partial H}{\partial x_\rho} \frac{\partial V_1}{\partial x_\rho} \frac{\partial V_2}{\partial x_\rho} \right)^2
\]
with \(x_{2\mu-1} = q_\mu, x_{2\mu} = p_\mu\) for \(\mu = 1,\ldots,(N+2)/4\), and \(x_{2\mu-1} = \tilde{q}_{\mu-M}, x_{2\mu} = \tilde{p}_{\mu-M}\) for \(\mu = (N+2)/4 + 1,\ldots,(N+2)/2\). In this case the number of lattice sites is \(M = (N+2)/4\). These equations are presently used to investigate the thermodynamics of two-component bosons mixtures in Ref. 16.

Final remarks.—In this paper we have proposed a geometric approach to measure thermodynamic observables within the microcanonical ensemble in classical Hamiltonian systems with \(K \geq 0\) independent conserved quantities. The method that we have shown is applicable also to systems with nonstandard Hamiltonians and with an arbitrary number of conserved quantities. As an example we have derived the formula of the temperature for a model that describes the superfluid dynamics of two-components bosons on an optical lattice.

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