Existence of a Potential for Dissipative Dynamical Systems

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It is shown that the existence of a potential is not a generic property of a continuous nonlinear dissipative system but requires the complete integrability of an associated Hamiltonian system.

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There has been an enormous interest recently in general properties of dissipative dynamical systems described by autonomous equations of the form

$$\dot{q}^\nu = K^\nu(q). \tag{1}$$

Henceforth, we assume that the real configuration space $-\infty < q^\nu < +\infty$ $(\nu = 1, \dots, f)$ is simply connected and that the dynamical system is stable in the sense that the Euclidian norm $\|q\|$ remains finite for all t and $t \to \infty$. We also assume that Eq. (1) does not admit a conservation law. One general problem associated with (1), which is of considerable physical interest, is whether it has a potential with respect to a certain given positive-semidefinite symmetric matrix $Q^{\nu\mu}$, which may be considered as a matrix of transport coefficients. For simplicity, we shall assume that $Q^{\nu\mu}$ is independent of q. Equation (1) is said to have a potential $\varphi(q)$ with respect to $Q^{\nu\mu}$ if there exists a single-valued, continuously differentiable and globally defined function $\varphi(q)$, bounded from below, which is stationary in the limit sets (attractors, repellors, saddle points, etc.) of Eq. (1) with respect to arbitrary infinitesimal variations of q, and which satisfies

$$K^\nu(q) = -\tfrac{1}{2} Q^{\nu\mu}\, \partial\varphi(q)/\partial q^\mu + r^\nu(q), \tag{2}$$

with

$$r^\nu(q)\, \partial\varphi(q)/\partial q^\nu = 0. \tag{3}$$

Examples of dissipative systems with potential are all macroscopic systems relaxing to thermodynamic equilibrium, where $Q^{\nu\mu}$ is the matrix of transport coefficients and φ is a thermodynamic potential. Nonequilibrium systems with a potential include models of lasers,[1-3] optical bistability,[4,5] or hydrodynamic instabilities, like the Bénard problem.[6,7] In addition, all one-dimensional systems of the form (1) and satisfying the assumptions made have a potential. Yet another general class with potential is formed by linear systems of the form (1). In all cases where a potential exists and where the matrix $Q^{\nu\mu}$ is positive definite, the potential is automatically a Lyapunov function of Eq. (1), as a result of Eqs. (2) and (3).

Even though it is generally believed that not all systems (1) have a potential, the general conditions for its existence have not been examined to our knowledge. It is the purpose of this Letter to present an investigation of this question. We show that the existence of a potential of (1) with respect to a matrix $Q^{\nu\mu}$ is not a generic property for a nonlinear system but requires the complete integrability of an associated Hamiltonian system. A second, equivalent condition for a potential is the existence of a continuous Markoff process $q^\nu(t, \eta)$, which reduces to the process (1) in the limit of vanishing noise $\eta = 0$, and whose steady-state distribution $W_\infty(q, \eta)$ defines a single-valued, continuously differentiable $\varphi(q) \not\equiv 0$, independent of η, bounded from below, by the limit $\varphi(q) = -\lim_{\eta\to 0} \eta \ln W_\infty(q, \eta)$. For systems where a potential is known to exist for thermodynamic reasons, this is the statement that the macroscopic description is the formal limit for Boltzmann's constant $k_B \to 0$ (or Loschmidt's number $\to \infty$) of the microscopic description of statistical mechanics.

We first prove the second condition. The Markoff process $q(\eta, t)$, which we associate with Eq. (1) and a symmetric nonnegative matrix $Q^{\nu\mu}$, is defined by the Fokker-Planck equation for the probability density $W(q, t)$:

$$\frac{\partial W}{\partial t} = -\frac{\partial}{\partial q^\nu} K^\nu(q) W + \frac{\eta}{2} \frac{\partial^2}{\partial q^\nu \partial q^\mu} Q^{\nu\mu} W. \tag{4}$$

For $\eta = 0$ it reduces to the process (1). Its steady-state distribution defines a function $\varphi(q, \eta)$ by $W_\infty(q, \eta) = N(\eta) \exp[-\varphi(q, \eta)/\eta]$, where N is a normalization constant. If $\varphi(q) = \lim_{\eta\to 0} \varphi(q, \eta)$ is a single-valued, continuously differentiable function bounded from below, it satisfies

$$K^\nu(q) \frac{\partial\varphi(q)}{\partial q^\nu} + \frac{1}{2} Q^{\nu\mu} \frac{\partial\varphi(q)}{\partial q^\nu} \frac{\partial\varphi(q)}{\partial q^\mu} = 0, \tag{5}$$

as follows immediately from Eq. (4). Equation

(5) is equivalent to Eqs. (2) and (3). Conversely, if a potential exists then the stationary solution of Eq. (4) in the limit $\eta \to 0$ is given by $W_\infty(q,\eta) \approx \exp[-\varphi(q)/\eta]$. Thus, the existence of such a stationary solution of Eq. (4) in the limit $\eta \to 0$ and of a potential $\varphi(q)$ are equivalent.

We now turn to the formal association of a Hamiltonian system with the system (1). This is done by interpreting (5) as a Hamilton-Jacobi equation where $\varphi(q)$ is the action and $p_\nu = \partial\varphi/\partial q^\nu$ are the momenta which are canonically conjugated to q^ν. The Hamiltonian which is given by the Hamilton-Jacobi theory,

$$H(q,p) = \tfrac{1}{2} Q^{\nu\mu} p_\nu p_\mu + K^\nu(q) p_\nu, \tag{6}$$

coincides with the Hamiltonian in the Martin-Siggia-Rose formalism[8] of the process (4). As in the latter formalism, the Hamiltonian structure of the dynamics has been achieved by the doubling of the number of variables. The Lagrangian associated with (6) can also be obtained from the functional integral which solves Eq. (4) for $\eta \to 0$.[3]

We now argue that the existence of a potential of (1) requires the complete integrability of the Hamiltonian dynamics defined by (6) for energy $H(q,p)\equiv 0$. As criterion for complete integrability we take the existence of smooth separatrices or "whiskered tori"[9] connecting the limit sets of Eq. (1) in the Hamiltonian system.

The $(2f-1)$-dimensional energy hypersurface $H\equiv 0$ in phase-space contains the f-dimensional invariant hyperplane S_0 defined by $p_\nu \equiv 0$ ($\nu = 1, \ldots, f$), on which the Hamiltonian dynamics reduces to Eq. (1). The union of the limit sets of Eq. (1), therefore, forms a set Γ on S_0. Γ has stable and unstable manifolds on S_0, which one obtains from Eq. (1). In addition, however, in the Hamiltonian system, there are stable and unstable manifolds of Γ transverse to S_0, on which not all p_ν vanish. The p_ν on these manifolds are locally given by

$$p_\nu = \partial\varphi(q)/\partial q^\nu, \quad \nu = 1, \ldots, f, \tag{7}$$

where $\varphi(q)$ is a special local solution of Eq. (5) which holds in a neighborhood of Γ and satisfies $\partial\varphi(q)/\partial \mathbf{q} = 0$ on Γ. We now have to distinguish two cases: (i) The Hamiltonian system is not integrable for $H=0$. This is the general case. It is then not possible to extend the different local pieces $\varphi(q)$ to a single-valued, continuously differentiable global solution, and a potential with the required properties does not exist. In particular, barring exceptions,[10] we have this case if the dissipative system (1) is chaotic, since (1) forms a subdynamics of the Hamiltonian system with $p_\nu \equiv 0$. (ii) The Hamiltonian system is integrable for $H=0$. In this case, the manifolds defined locally by Eq. (7) can be extended to global smooth separatrices transverse to S_0. If Γ consists of several attractors and repellors, the smooth separatrices transverse to S_0, which connect them, form one part of "whiskered tori," the other parts of which are formed by S_0. (For a concrete example see Fig. 1.) This establishes the integrability of the Hamiltonian system at $H=0$ as a necessary condition for the existence of a potential. It is not a sufficient condition, however, since a potential can only be constructed if Eq. (5) is soluble by a global *single-valued* function $\varphi(q)$ which satisfies the boundary condition $\partial\varphi/\partial\mathbf{q}=0$ on Γ. We have shown, therefore, that dissipative systems with a potential are special. If they are only slightly perturbed in an arbitrary way, the smooth separatrices defined by Eq. (7) are destroyed and a potential ceases to exist. This is our central result.

As a concrete example, we consider the dynamical system

$$\dot{x} = \epsilon[x - x^3 + f(x)\cos y], \quad \dot{y} = \omega, \tag{8}$$

and the matrix

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

The Hamiltonian (6) is given by

$$H = \tfrac{1}{2} p_x^{\,2} + p_x \epsilon[x - x^3 + f(x)\cos y] + \omega p_y. \tag{9}$$

The integrability of the Hamiltonian dynamics at $H=0$ is most conveniently studied by using the Poincaré cross section of the three-dimensional

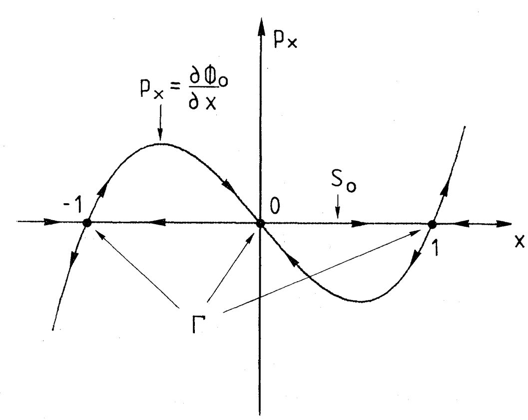

FIG. 1. Poincaré cross section of S_0, Γ, and the stable and unstable manifolds of Γ for the model (8) with $f(x)=0$.

energy hypersurface at $y=0$. For $f(x)\equiv 0$ the system has a potential $\varphi_0=-\epsilon(x^2-x^4/2)$, which is easily obtained from Eq. (5). The intersection with the (x, p_x) plane of the manifold S_0, the set Γ, and the separatrix formed by $p_x=\partial\varphi_0/\partial x$ are shown in Fig. 1. For $f(x)\neq 0$, Eqs. (8) have, in general, no potential with respect to Q. We have carried out a detailed analysis of this case by numerical and analytical methods, which will be published elsewhere.[11] Here, we mention only some results which are pertinent to the present discussion. In Fig. 2 we show the numerical evaluation near $x=0$ of the unstable manifold of the point $P=(1, 0)$ for the case $f(x)=a(x-x^3)$, $a=\epsilon=0.1$, $\omega=1$, which illustrates that this manifold has ceased to form a smooth separatrix and the Hamiltonian system has ceased to be completely integrable. We present also the result of an analytical investigation of the same case which is based on (a) an expansion in ϵ to third order and (b) an expansion in a to first order. The result of the expansion in a allows us to understand analytically the onset of the oscillations of the unstable manifold of the point P near $p_x=0, x=0$. We found that the oscillations are produced by terms in $\varphi(q)$ which are not analytic in ϵ for $\epsilon\to 0$. The expansion in ϵ, on the other hand, lacks all these nonanalytical terms and, therefore, does not describe the oscillations of the manifold. Instead, the ϵ expansion yields an analytical function

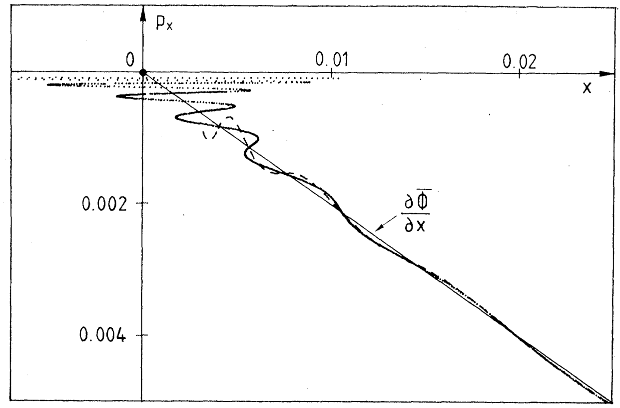

FIG. 2. Poincaré cross section of the unstable manifold of ($p_x=0$, $x=1$) near $x=0$ of the model (8) for $f(x)=ax(1-x^2)$, $\epsilon=a=0.1$, $\omega=1$. Analytical approximation to first order in a (dashed line), and the unstable manifold derived from the approximate potential $\overline{\varphi}(x,y)$ of Eq. (10) (full line) are also shown.

$$\overline{\varphi}(x, y)=-\epsilon(x^2-x^4/2)+2\epsilon^2 ax^2(1-x^2)^2\sin y + \epsilon^3[ax^2(1-x^2)^2(1-3x^2)(a\cos 2y-4\cos y)+a^2x^4(3-4x^2+3x^4/2)]+O(\epsilon^4). \tag{10}$$

In Fig. 2 we compare the approximation provided by Eq. (10) for $\epsilon=0.1$ with the unstable manifold of $P=(1, 0)$ in the very close vicinity of $P_0=(0,0)$, where the approximation is seen to break down. However, outside this region, the unstable manifold of P is very well approximated by $p_x=\partial\overline{\varphi}/\partial x$. A similar comparison could be made with the stable manifold of P_0. Here the approximation breaks down only in a tiny neighborhood of P. Thus, $\overline{\varphi}(x, y)$ is a good approximate potential of Eqs. (8). Approximate potentials for optically bistable systems[5] and for dissipative systems with a single attractor[12] have been constructed earlier along similar lines.

We conclude with some general remarks on our main result. The fact that one-dimensional systems and linear dissipative systems always have a potential is, of course, consistent with our result, since Hamiltonian systems with one degree of freedom or with quadratic Hamiltonians are completely integrable. The fact that dynamical systems in equilibrium thermodynamics always have a potential has deeper reasons. There are special constraints on the form of the Hamiltonian (6) in thermodynics, ensuring its integrability, which follow from microscopic reversibility and the fact that the macroscopic variables q^ν transform simply (even or odd) under time reversal.

In general, $K^\nu(q)$, $Q^{\nu\mu}$, and $W_\infty(q, \eta)$ in Eq. (4) are connected by the "potential conditions"[13]

$$K^\nu(q)=-\tfrac{1}{2}Q^{\nu\mu}\,\partial\varphi(q, \eta)/\partial q^\mu+r^\nu(q, \eta),$$
$$\eta\,\partial r^\nu(q, \eta)/\partial q^\nu-r^\nu(q, \eta)\,\partial\varphi(q, \eta)/\partial q^\nu=0. \tag{11}$$

Microscopic reversibility implies that $r^\nu(q, \eta)$ is given by that part of $K^\nu(q)$ which transforms like $\dot{q}^\nu$ under the microscopically defined transformation of time reversal, and $r^\nu(q, \eta)$ and $\varphi(q, \eta)$ must be independent of η as $K^\nu(q)$ is independent of η, since η-dependent terms with opposite parity under time reversal cannot cancel. The limit $\eta\to 0$ is, therefore, superfluous in this case and $\varphi(q, \eta)=\varphi(q)$ is a single-valued, continuously differentiable globally defined function bounded from below because of its relation with $W_\infty(q, \eta)$. It satisfies Eq. (5) automatically.

For general nonlinear systems Eqs. (11) can still be written down, but $r^\nu(\boldsymbol{q}, \eta)$ must now be allowed to depend on η. Formally, it is even possible to *define* a new transformation of time reversal, different from the microscopically defined transformation, according to which $r^\nu(q, \eta)$ is still the part of $K^\nu(q)$ transforming like $\dot{q}^\nu$ ("hidden detailed balance"[14]). However, this new transformation of time reversal, in general, depends on η by definition and, therefore, it cannot be used to rule out a dependence of $r^\nu(q, \eta)$ on η. Hence, no general conclusions on the behavior of the limit $\eta \to 0$ of $r^\nu(q, \eta)$ and $\varphi(q, \eta)$ is possible.

If the system has a potential one may usefully generalize the formalism of thermodynamics. In this paper we have shown that this case is exceptional for a nonlinear dynamical system, but the special example we considered has also revealed that approximate potentials may still provide a very accurate description even in cases where an exact potential does not exist.

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[10]There is the possibility that the Hamiltonian system (6) is separable in certain coordinates into an integrable part and a nonintegrable one. Then our arguments can be applied to the integrable part alone and may lead to a solution of Eq. (5) which satisfies the boundary condition $\partial\varphi/\partial q = 0$ on Γ and depends on the coordinates of the integrable part only.

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