Planar Curve Representation of Many-Body Systems and Dynamics

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(Received 11 July 1996)

A method is introduced to represent many-body systems of arbitrary dimensionality by planar curves. The positions and momenta of the particles are the parameters of a time-dependent nonlinear transformation, which maps the many-body dynamics of the real system to the motion of the curve. The description of the system as a point in a multidimensional phase space is thus replaced by a two-dimensional continuous line. Expressions for the curvature along the curve and the dynamic structure factor are obtained. The formulation holds for Hamiltonian and non-Hamiltonian systems, and two explicit examples are analyzed: harmonic oscillators and a quadratic system. [S0031-9007(97)02340-5]

PACS numbers: 03.20.+i

An important theme in scientific studies is the interpretation and understanding of various physical theories and formalisms in terms of geometry. This theme dominated the studies of giants such as Euclides, Riemann, Minkovsky, and Einstein. One manifestation of this idea in contemporary science, which focuses much attention in many fields, is the relation of partial differential equations to symmetry groups and geometry. Another related aspect concerns the shape and motion of curves and surfaces, which, besides its theoretical relevance, is also of practical importance where the dynamics of interfaces and fronts is of interest. Examples abound in nature and in technological applications: solidification processes, shock waves, kinematics of polymers, and motion of line vortices, to name a few.

Here a different aspect of the usefulness of geometrical representation is explored: the possibility to described many-body systems (MBS) as planar curves. The formalism to be developed here has several intriguing aspects: First, it enables a low-dimensional visualizable description of systems. Second, it helps representing the system's dynamics as a moving curve, which in many cases is more accessible to both numerical and analytical study. Third, the correspondence between the distribution of the particles of the MBS and the morphology of the curve gives a new handle on statistical analysis of multiparticles physical systems. Fourth, in many circumstances a continuous two-dimensional curve representation of a system of N particles has an advantage over the traditional view of a system as a point moving along a trajectory in some huge $6N$-dimensional phase space. An interesting application of this formalism is to communication, where the curve's configuration can represent a complicated data and can be used as an efficient method for data reduction, storage, and presentation. In this context, the curve's dynamics is a sequence of successive time step configurations that correspond to a series of information strings. This formalism is applicable to any dynamical system, Hamiltonian and non-Hamiltonian, describing a set of time-dependent variables. Two examples are explicitly discussed below.

Consider a MBS consisting of two-species particles a and b of equal numbers. For simplicity, the systems discussed here will be assumed to have an even number of particles, but this does not limit the formalism; an odd number of particles can be augmented by a fictitious extra particle with a predesigned behavior. In systems of only one species one can generate an image of all the particles, which are then treated as the second species, as detailed below. The system is presumed to follow a set of dynamical equations

$$\dot{q}_{\alpha,n} = g_{\alpha,n}; \quad n = 1,2,\ldots,N; \quad \alpha = a,b\,. \tag{1}$$

Denoting by $p_{\alpha,n} = m\dot{q}_{\alpha,n}$ the momenta of the particles, we can construct a new set of equations by differentiating the set (1) and replacing the momenta for the derivatives of the positions on the right-hand side:

$$\dot{p}_{\alpha,n} = h_{\alpha,n}(\vec{q},\vec{p})\,. \tag{2}$$

If the system is Hamiltonian, for example, the two sets $\vec{g}$ and $\vec{h}$ can be cast in the form of Hamilton's equations (see below), which means that Eqs. (1) and (2) are derivable from a scalar function H. Our goal now is to represent the MBS *at any moment in time* by a planar curve whose properties are uniquely determined by the momentary values of the particles' positions and momenta. The representative curve is a complex function $\gamma(s,t)$ whose real and imaginary parts denote, respectively, the x and y coordinates of the curve in a complex plane. The parameter s runs along the curve and takes on values between 0 and 2π, and t denotes time. It is convenient to describe the curve as the limit of a function $F(z,t)$, which is defined over the entire complex plane. To this end we consider the following conformal meromorphic map from the outside of the unit circle in the complex z plane onto the outside of a simply connected (Jordan) curve in ζ complex plane $\zeta = u + iv$,

$$\frac{dF}{dz} = F' = \prod_{n=1}^{N} \frac{z - Q_{a,n}}{z - Q_{b,n}}\,, \tag{3}$$

where $Q_{\alpha,n} = q_{\alpha,n} + ip_{\alpha,n}$. For brevity, denote in the following $Q_{a,n}$ by Z_n and $Q_{b,n}$ by P_n. The curve is recovered from F by taking the limit $\gamma(s,t) = \lim_{z\to e^{is}} F(z,t)$. We can now study the kinetics of the map by following the motion of the particles. Integrating Eq. (3) yields

$$F = z + \sum_{n=1}^{N} C_n \ln(z - P_n), \qquad (4)$$

where the coefficients C_n are the residues of the product in (3) at the points $z = Q_{b,n}$,

$$C_n = (P_n - Z_n) \prod_{m'=1}^{N} \frac{P_n - Z'_m}{P_n - P'_m}; \quad m' \neq n .$$

These coefficients are independent of the spatial coordinate z but can vary with time. The map is conformal-meromorphic, and we require therefore that it possess no branch far from the unit circle, viz., $\oint_\Gamma F d_z = 0$, where Γ is a contour at $z \to \infty$. Upon integrating Eq. (3) it can be readily found that this condition implies

$$\sum_{n=1}^{N} C_n = 0, \qquad (5)$$

which can be shown [1] to be equivalent to requiring that

$$\sum_{n=1}^{N} Z_n = \sum_{n=1}^{N} P_n . \qquad (6)$$

It would be appropriate to term condition (6) "dipolar neutrality" because the different species can be regarded as positive and negative charges of a charge neutral system. Equation (6) then represents the vanishing of the *dipolar* sum of N two-dimensional vectors each extending from a positive particle to a negative, with the pairs chosen arbitrarily. The conditions of charge and dipolar neutrality are necessary for mapping the unit circle in the z plane onto a simply-connected curve in the ζ plane. Before continuing, let us make precise the definition of the second species in a one-species system: Given K particles, define a new particle Z_0 whose dynamics are such that the dipolar sum always vanishes, $\sum_{n=0}^{K} Z_n = 0$. Now define $K + 1$ image particles by $P_n = -Z_n$ as the second species (poles). The new system has $2K + 2$ particles that can be described by the present formalism.

The description of the curve in Fourier modes is obtained as follows: Using relation (5), expand relation (4) in powers of z,

$$F = z + \sum_{k=1}^{\infty} d_k z^{-k}; \quad d_k = \frac{1}{k} \sum_{n=1}^{N} C_n P_n^k , \qquad (7)$$

and take the limit $z \to \exp(is)$. Note that the quantity d_{k+1} can be regarded as the kth moment of the distribution of P_n, with (complex) weight $C_n P_n$. We point out that the time dependence of the curve enters only through the coefficients $d_k(t)$. The form of $F(z)$ in (7) is called univalent, a class of functions whose properties are well known. In particular, for such a function to map the unit circle onto a *simply-connected* curve, it is sufficient that the coefficients d_k satisfy the Bieberbach requirement

$$|d_K| \le 2/(k + 1). \qquad (8)$$

This condition may be, however, too strong, an issue that will be addressed elsewhere [2]. The above is the bare result of this paper: the mapping of a discrete MBS onto an equivalent *continuous* planar curve. Before we continue we note that the MBS can be recovered from the kinetics of the curve: Given the equation for $F(z,t)$, $\dot{F} = \mathcal{F}$, where $\mathcal{F}$ is a function of F, ∇F, z, etc., perform the following Cauchy-integral along a contour that contains $\Gamma_n = Z_n$ or P_n,

$$\frac{1}{2\pi i} \oint_{\Gamma_n} \dot{F}'/F' dz = \frac{1}{2\pi i} \oint_{\Gamma_n} \mathcal{F}'/F' dz .$$

This yields the equation of motion of that particle, $\dot{\Gamma}_n (= -\dot{Z}_n$ or $\dot{P}_n)$. Thus the seeming increase in dimensionality (finite $\to$ infinite) is an artifact of the nonlinear transformation, and the continuous description contains, in fact, no information beyond the original system. One can now translate any of the quantities that are useful for the study of MBS to the curve representation and vice versa. For example, a useful measure along the curve is the curvature expressed as a function of the parameter s. A straightforward calculation shows that, in terms of the positions and momenta of the particles, the curvature is given by

$$\kappa(s) = \frac{1}{|F'|} \left\{ 1 + \mathrm{Re} \sum_{n=1}^{N} \sum_{\alpha} \left[\frac{\epsilon_\alpha}{1 - Q_{a,n} e^{-is}} \right] \right\}, \qquad (9)$$

where $\epsilon_\alpha = 1(-1)$ when $\alpha = a(b)$, represents the "charge" of the particle. Thus the value of the curvature at each point s along the planar curve is uniquely determined by the particular configuration of the particles Q_α, making the planar curve description a one-to-one representation of the particles configuration.

Another quantity is the curve's dynamic structure factor defined through

$$S(q,\omega) = \int \frac{ds ds' dt dt'}{(2\pi)^4} \gamma(s,t) \gamma(s',t') e^{iq(s-s') + i\omega(t-t')}. \qquad (10)$$

Using Eq. (7) in (10) we find that

$$S(q,\omega) = \tilde{d}_q(\omega) \tilde{d}_q(-\omega), \qquad (11)$$

where $\tilde{d}_k(\omega)$ is the Fourier transform of $d_k(t)$. These two quantities can also be used for a statistical analysis of the curve's shape and its correspondence to the initial system's statistics.

Next we want to derive the relation between the dynamics of the particles and the motion of the curve. Clearly, the evolution of the curve is dependent on the kinetics of the particles through their equations of motion, (1) and (2). The evolution of the map $F(z,t)$ is governed by the partial differential equation

$$\dot{F} = \sum_{n=1}^{N} \left[\dot{C}_n \ln(z - P_n) - C_n \frac{\dot{P}_n}{z - P_n} \right]. \qquad (12)$$

Using their definition, the values of $\{\dot{C}\}$ can be expressed in terms of $\{\dot{Q}_\alpha\}$, which in turn are given by the functions $\vec{g}$ and $\vec{h}$ in Eqs. (1) and (2). Thus the entire sum on the right-hand side of (12) can be expressed in terms of only the momentary positions and momenta of the particles, $\dot{F} = \dot{F}(\{Z\},\{P\})$. Taking again the limit $z \to \exp(is)$ in $\boldsymbol{F}$ gives the required equation of motion of $\gamma(s,t)$, which establishes the correspondence between the curve and the MBS dynamics.

Hamiltonian dynamical systems form a special class of MBS, where $\vec{g}$ and $\vec{h}$ are related by a scalar energy function. Consider a system of two $\boldsymbol{N}$-particle species with the Hamiltonian $H(\{q\},\{p\})$ and canonical variables $\{q_{a,n}\}$, $\{q_{b,n}\}$, $\{p_{a,n}\}$, $\{p_{b,n}\}$. The dynamics follow Hamilton's equations:

$$\dot{q}_{\alpha,n} = \frac{\partial H}{\partial p_{\alpha,n}}; \quad \dot{p}_{\alpha,n} = -\frac{\partial H}{\partial q_{\alpha,n}}. \tag{13}$$

In terms of the complex variables $Q_{\alpha,n} = q_{\alpha,n} + ip_{\alpha,n}$, Hamilton's equations can be written as

$$\dot{Q}_{\alpha,n} = -i\partial H/\partial Q^*_{\alpha,n},$$

where $Q^*_\alpha = q_\alpha - ip_\alpha$ is the complex conjugate of Q_α. Substituting relations (13) in (1) and (2), and using the above formulation, gives the dynamics of the equivalent curve. Since Hamilton's equations, (13), hold in any dimension with the different spatial components of the positions and momenta treated as independent degrees of freedom, then the present formalism maps *any d-dimensional system* into a planar curve.

For illustration, let us analyze two examples: the first, a system of (canonical) harmonic oscillators. For clarity, I focus on four particles undergoing simple harmonic oscillations in one dimension:

$$H = \frac{1}{2}\sum_{\alpha=a,b}\sum_{n=1}^{2}[p^2_{\alpha,n} + q^2_{\alpha,n}], \tag{14}$$

where the particles (and their dynamics) are symmetrical about the origin, as shown in Fig. 1. The generalization to higher dimensions and to more particles is straightforward. The trajectories are

$$q_{\alpha,n} = A_{\alpha,n}[x_{\alpha,n} + \cos(t + \theta_{\alpha,n})],$$
$$p_{\alpha,n} = \dot{q}_{\alpha,n}, \tag{15}$$

where $A_{\alpha,n}$, $x_{\alpha,n}$, and $\theta_{\alpha,n}$ are, respectively, the amplitudes, the normalized central positions, and the phases of the oscillations. Since the $\boldsymbol{b}$ oscillators are the mirror image of the $\boldsymbol{a}$'s at any time, the system is automatically charge and dipolar neutral, and we have $A_{\alpha,1} = A_{\alpha,2} \equiv A_\alpha$, $x_{\alpha,1} = -x_{\alpha,2} \equiv x_\alpha$, and $\theta_{\alpha,1} = \theta_{\alpha,2} + \pi \equiv \theta_\alpha$. The locations of the poles and the zeros are shown schematically in Fig. 1 both in the (1D) real space and in the complex q-p plane. Using Eq. (4), we find that $C_1 = (P_1^2 - Z_1^2)/2P_1 = -C_2$, and

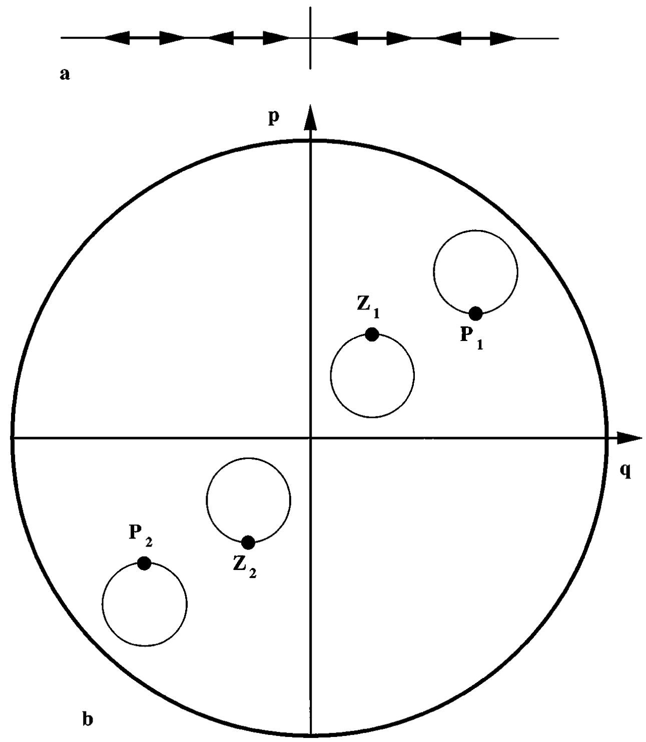

FIG. 1. A system of four harmonic oscillators in one dimension: (a) in real space, and (b) in the complex plane.

the explicit curve trajectory is given by

$$\gamma(s,t) = e^{is} + \frac{P_1^2 - Z_1^2}{2P_1}\ln\frac{e^{is} - P_1}{e^{is} + P_1}. \tag{16}$$

This curve is an ellipse that oscillates with time. The Fourier representation follows from (16):

$$d_k = (Z_1^2 - P_1^2)P_1^{k-1}/k, \quad k \text{ odd},$$
$$d_k = 0, \quad k \text{ even}. \tag{17}$$

From this expression it is straightforward to compute $\tilde{d}_q(\omega)$ and, using (11), $S(q,\omega)$, which turns out to consist of a finite number of delta functions. The curvature along the curve is given in terms of the oscillators Z_1 and P_1 as

$$\left|\frac{e^{2is} - P_1^2}{e^{2is} - Z_1^2}\right|\left\{1 + 2\mathrm{Re}\left[\frac{e^{is}}{e^{2is} - Z_1^2} - \frac{e^{is}}{e^{2is} - P_1^2}\right]\right\}. \tag{18}$$

As a less straightforward example consider a quadratic dissipative dynamical system

$$\dot{A} = -1.55A^2/3A_0 + 0.2AB/3B_0,$$
$$\dot{B} = -5.5B_0A^2/3A_0^2 + 0.1B^2/3B_0, \tag{19}$$

with the initial conditions $A(t=0) = A_0 \le 1/\sqrt{1.2025}$ and $B(t=0) = B_0 \le 1/\sqrt{4.24}$. The evolution of this system follows:

$$A = A_0[2/(1 + 0.3t) - 1/(1 + 0.15t)],$$
$$B = B_0[11/(1 + 0.3t) - 10/(1 + 0.15t)]. \tag{20}$$

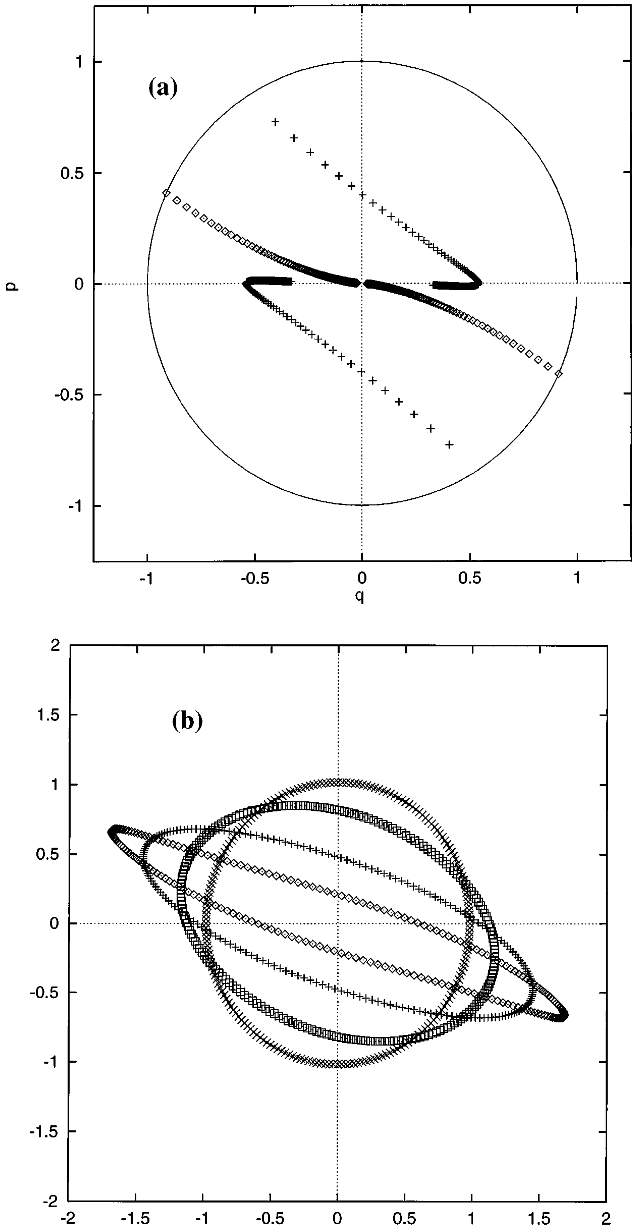

FIG. 2. A quadratic system of two variables and their mirror images: (a) the particles trajectories in the q-p plane; (b) the corresponding curve evolution.

The assigned particles are $Z_1 = A + i\dot{A} = -Z_2$ and $P_1 = B + i\dot{B} = -P_2$, and the curve representing this system is then given by Eq. (16). The coefficients d_k are given by (17) and the curvature along the curve is

$$\left| 1 + \frac{Z_1^2 - P_1^2}{e^{2is} - Z_1^2} \right| \times \left[1 + 2\mathrm{Re}\, \frac{Z_1^2 - P_1^2}{e^{2is} - (Z_1^2 + P_1^2) + P_1^2 Z_1^2 \exp^{-2is}} \right]. \tag{21}$$

The trajectories of the particles are shown in Fig. 2(a) and the corresponding curve evolution in Fig. 2(b). With time, $\gamma(s)$ changes from an elongated twisted form (at $t = 0$) to an ellipse, while slowly rotating in the process. As $t \to \infty$ the curve tends to a circle due to the decaying solution.

To summarize, it was shown that any d-dimensional many-body system, confined to within a finite support, can be represented by a closed Jordan curve in a complex plane. The correspondence between the dynamics of the particles of the MBS and the motion of the curve was established. It was shown that an explicit expression for the curvature along the curve in terms of the momentary distribution of the particles can be given, and the dynamic structure factor was derived. The application to Hamiltonian and non-Hamiltonian systems was illustrated with two examples that were analyzed explicitly. It is emphasized that the dynamics of the curve, which are governed by one partial differential equation (12), is completely equivalent to the *finite* set of discrete equations $\vec{g}$ and $\vec{h}$, and therefore should be useful in analyzing many-body systems in general. It should be noted that the conformal map used here is only one of many that can be employed to transform a MBS to a curve, which makes this formalism quite flexible. The reduction of the description to two dimensions, rather than the traditional huge phase space, is expected to lead to many advantages, in particular where statistical analyses are relevant. The application of statistical mechanical tools to Hamiltonian systems within this formalism is currently one of the issues being explored. For practical purposes, the planar curve representation can help in data reduction and storage, two key issues in today's computational-oriented technology. It can also be used for visual comparison between systems and for pattern recognition by devices using visual-like processes.

This work was funded in part by IOTA Inc., VA.

[1] R. Blumenfeld, Phys. Rev. E **50**, 2952 (1994); R. Blumenfeld and R.C. Ball, Phys. Rev. E **51**, 3434 (1995).
[2] R. Blumenfeld, "Curve-Representation of Noise" (to be published).