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ON THE STOCHASTIC MODELING OF RIGID BODY SYSTEMS WITH APPLICATION TO POLYMER DYNAMICS*

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Abstract. The stochastic equations of motion for a system of interacting rigid bodies in a solvent are formulated and studied. Three-dimensional bodies of arbitrary shape, with arbitrary couplings between translational and rotational degrees of freedom, as arise in coarse-grained models of polymers, are considered. Beginning from an Euler–Langevin form of the equations, two different, properly invariant, Hamilton–Langevin forms are derived and studied together with various associated measures. Under different conditions depending on the choice of rotational coordinates, the canonical measure is shown to be a stationary solution of an associated Fokker–Planck equation and to always factorize into independent measures on configuration and velocity spaces. Explicit expressions are given for these measures, along with a certain Jacobian factor associated with the three-dimensional rotation group. When specialized to a fully coupled, quadratic model of a stiff polymer such as DNA, our results yield an explicit characterization of the complete set of model parameters.

Key words. Euler–Langevin equations, Hamilton–Langevin equations, stationary measures, polymer modeling

AMS subject classifications. 60H10, 70E99, 70H05, 82C22, 82C31

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1. Introduction.

The mechanical properties of polymers in a solvent can be studied through the use of various types of models, for example, detailed atomistic-type models, coarse-grained chain-type models built from bead or link elements, and continuous rod-type models based on the classic theory of elasticity [5, 11, 13, 14, 21, 33, 38, 43, 47, 54]. These types of models resolve polymer properties to different levels of detail, possess different practical limitations, and together provide a means to explore properties at different scales. At short length scales where local structural features are important, atomistic-type models are typically appropriate, and a solvent is usually included explicitly in the model. At long length scales where local features average out, homogeneous chain- or rod-type models are typically appropriate, and a solvent is usually included implicitly through viscous and stochastic loads. Resolving polymer properties at intermediate scales, for example, the biologically important scale of tens to hundreds of basepairs in the case of DNA, poses special problems. Such scales are prohibitively expensive for detailed atomistic-type models, yet often involve important local features that are below the resolution of the homogeneous models typical in polymer physics.

A class of models that are particularly well suited for intermediate scales are those based on interacting, three-dimensional rigid bodies. Compared to detailed atomistic models, rigid body models are coarse-grained and consequently simpler to parameterize, simulate, and understand. Compared to homogeneous chain-type models built

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from bead or link elements, rigid body models are more detailed and consequently better adapted to represent local features. Whereas the beads or links in a chain-type model are typically meant to correspond to segments of polymer consisting of several monomers, the bodies in a rigid body model are meant to correspond to individual monomer units, such as bases or basepairs in the case of DNA. Moreover, while interactions between beads and links in a chain-type model represent average interactions over several monomers, interactions between bodies in a rigid body model can represent local molecular interactions between specific monomer units. In the case of DNA, rigid body models offer a promising approach to understand various local structural features, such as sequence-dependent curvature and deformability, as have been investigated by various authors [6, 9, 20, 42, 46, 48]. The continuum limit of rigid body models lead naturally to inhomogeneous rod models of the Kirchhoff or Cosserat types, whose mathematical properties are well understood [1] and whose minimum energy configurations have been successfully used in various recent investigations of DNA [15, 35, 52, 53].

In this article, we outline a stochastic rigid body model for a polymer in a solvent and study its mathematical properties. We consider a system of multiple, interacting, three-dimensional rigid bodies of arbitrary shape, with arbitrary couplings between their translational and rotational degrees of freedom, immersed in a solvent which is modeled implicitly through viscous and stochastic loads. We begin with an Euler–Langevin model of a single rigid body and use the rules of stochastic calculus to derive different forms of the equations of motion. We show that the equations can be phrased in both canonical and noncanonical Hamilton–Langevin forms and show that each form is natural in the sense that each is invariant under an arbitrary change of configuration variables. A unique feature of our treatment is that translational and rotational degrees of freedom are fully coupled not only through the viscous and stochastic loads but also through a potential defined on the space of translations and rotations. Whereas coupling among all degrees of freedom is a natural and well-studied case in the modeling of point masses [7, 23, 27], it has received little attention in the modeling of rigid bodies, where motions have traditionally been modeled in the absence of a potential defined on the three-dimensional rotation group [34, 39].

We study the classic canonical measure for our stochastic rigid body model and examine the implications of different choices of rotational coordinate charts. For concreteness, we focus attention on two standard types: Euler angle charts, for which the coordinate domain is bounded and some coordinates are cyclic in an appropriate sense (see section 3), and Cayley charts, for which the coordinate domain is unbounded and all coordinates are acyclic. We outline a form of the celebrated fluctuation-dissipation theorem [29], which provides conditions under which the canonical measure is stationary under the flow of the canonical Hamilton–Langevin equations, or equivalently is a steady-state solution of the associated Fokker–Planck equation [18, 31, 45, 49], and show that the conditions which guarantee stationarity impose different restrictions on the translational and rotational components of the potential energy. Whereas a growth condition is necessary in the translational coordinates, it is not necessary in the rotational ones, even if the rotational coordinate domain is unbounded. Moreover, whereas periodicity conditions are necessary when the rotational coordinate domain is bounded, they are not necessary when the domain is unbounded. Implications of these conditions in the modeling of bodies with unrestrained and strongly restrained rotational degrees of freedom are discussed.

Furthermore, we study the factorability of the canonical measure, which property is crucial in various applications. Due to the nonseparability of the rigid body Ham-

iltonian in canonical variables, the canonical measure does not explicitly factor into independent measures over the configuration and conjugate momenta spaces. However, we show that, by a simple change of variables on the momenta, the measure can always be explicitly factored into certain independent, canonical measures over the body configuration and velocity spaces, the product of which is stationary under the flow of the noncanonical Hamilton–Langevin equations. The exact, explicit canonical configuration measure derived here contains a Jacobian factor associated with the three-dimensional rotation group. We show that this factor has an elegant geometrical interpretation as the determinant of a velocity structure matrix. Moreover, just as with the canonical measure on phase space, we show that the derived measure on configuration space is invariant under an arbitrary transformation of this space, which implies that the canonical configuration measure is intrinsic to the system. This invariance property depends crucially on the Jacobian factor.

We then extend our results from a single body to an arbitrary system of interacting rigid bodies. We describe how all results pertaining to the Hamiltonian form of the equations of motion and the associated canonical measures on phase, configuration, and velocity space carry over to systems. As an example application, we specialize our results to a rigid body model of a topologically linear polymer. We consider the case in which the potential energy of the system is a general quadratic function of a natural set of internal coordinates describing the relative, three-dimensional displacements and rotations between bodies. We outline the internal coordinates for the system and derive explicit forms for the associated canonical measures on the various spaces. Furthermore, we derive relations which characterize the complete set of potential energy and mass parameters of the model in terms of the expected or average values of certain state functions, or ratios thereof. Although the potential energy is quadratic, the canonical configuration measure is non-Gaussian due to a Jacobian factor. Thus our characterization relations can be viewed as generalizations of the usual Gaussian relations and provide a tool for parameter estimation from stationary time series and other types of data.

The presentation is organized as follows. In section 2, we outline a basic Euler–Langevin model for a rigid body in a solvent. In section 3, we derive various Hamilton–Langevin formulations of the model and establish important invariance properties. In section 4, we introduce the associated canonical measure for the model, study conditions which guarantee that it is stationary, factorize it into independent measures on the configuration and velocity spaces, and show that each measure is invariant in accordance with the invariance of the Hamilton–Langevin equations. In section 5, we extend our results to a system of rigid bodies with arbitrary interactions. In section 6, we specialize our results to a quadratic model of a topologically linear polymer and characterize the complete set of model parameters. In section 7, we summarize our results and conclusions.

2. Stochastic rigid body model. Here we outline our basic model for a rigid body subject to viscous, conservative, and stochastic loads. We do not attempt to justify these equations from a more refined theory. Instead, we simply postulate them and study the consequences. The model outlined here can be viewed as a generalization to a rigid body of the classic Langevin model for a particle in a potential field. For treatments of the particle case see [8, 18, 23, 45], and for general background on rigid body mechanics see [3, 19, 26].

2.1. Basic kinematics, balance laws. We consider an arbitrary rigid body whose configuration is defined by a vector $\boldsymbol{r}_0$ and an orthonormal frame $\{\boldsymbol{d}_i\}$ $(i =$

$1, 2, 3$). The vector $\boldsymbol{r}_0$ describes the position of the center of mass, whereas the frame $\{\boldsymbol{d}_i\}$ is fixed in the body and describes its orientation relative to a frame $\{\boldsymbol{e}_i\}$ fixed in space. The kinematics of the body are encapsulated in the relations

$$\dot{\boldsymbol{r}}_0 = \boldsymbol{v}_0, \qquad \dot{\boldsymbol{d}}_i = \boldsymbol{\omega} \times \boldsymbol{d}_i, \tag{2.1}$$

where $\boldsymbol{v}_0$ is the velocity of the center of mass, $\boldsymbol{\omega}$ is the angular velocity of the body frame, an overdot denotes a derivative with respect to time, and $\times$ denotes the standard vector product. The linear momentum $\boldsymbol{p}$ and angular momentum $\boldsymbol{\pi}_0$ of the body about its center of mass are defined by

$$\boldsymbol{p} = m\boldsymbol{v}_0, \qquad \boldsymbol{\pi}_0 = \boldsymbol{I}\boldsymbol{\omega}, \tag{2.2}$$

where m is the total mass and $\boldsymbol{I}$ is the symmetric, positive-definite rotational inertia tensor with respect to the center of mass, which in general is configuration, and therefore time, dependent. When the body is acted upon by a system of loads with resultant force $\boldsymbol{f}$ and resultant torque $\boldsymbol{\tau}_0$ about the center of mass, the balance laws for linear and angular momenta take the simple form

$$\dot{\boldsymbol{p}} = \boldsymbol{f}, \qquad \dot{\boldsymbol{\pi}}_0 = \boldsymbol{\tau}_0. \tag{2.3}$$

2.2. General kinematics, balance laws. In some applications, it is desirable to refer the angular momentum of the body and the resultant loads to a general, body-fixed reference point $\boldsymbol{r}$ rather than the center of mass $\boldsymbol{r}_0$, whose location in the body may not be known explicitly. Thus, let $\boldsymbol{r} = \boldsymbol{r}_0 - \boldsymbol{c}$, where $\boldsymbol{c}$ is a vector that is fixed in the body. Substituting this relation into (2.1) and noting that $\dot{\boldsymbol{c}} = \boldsymbol{\omega} \times \boldsymbol{c}$ because $\boldsymbol{c}$ is fixed in the body, we find that the kinematical relations take the form

$$\dot{\boldsymbol{r}} = \boldsymbol{v}, \qquad \dot{\boldsymbol{d}}_i = \boldsymbol{\omega} \times \boldsymbol{d}_i, \tag{2.4}$$

where $\boldsymbol{v} = \boldsymbol{v}_0 - \boldsymbol{\omega} \times \boldsymbol{c}$. Notice that $\boldsymbol{v}$ is the velocity of the reference point and that the linear momentum in (2.2) becomes $\boldsymbol{p} = m(\boldsymbol{v} + \boldsymbol{\omega} \times \boldsymbol{c})$. Moreover, let $\boldsymbol{\pi}$ and $\boldsymbol{\tau}$ denote the angular momentum and resultant torque about the reference point, which are defined as

$$\boldsymbol{\pi} = \boldsymbol{\pi}_0 + \boldsymbol{c} \times \boldsymbol{p}, \qquad \boldsymbol{\tau} = \boldsymbol{\tau}_0 + \boldsymbol{c} \times \boldsymbol{f}. \tag{2.5}$$

Substituting (2.5) into (2.3) and again using the fact that $\dot{\boldsymbol{c}} = \boldsymbol{\omega} \times \boldsymbol{c}$, we find that the balance laws of linear and angular momenta take the form

$$\dot{\boldsymbol{p}} = \boldsymbol{f}, \qquad \dot{\boldsymbol{\pi}} = (\boldsymbol{\omega} \times \boldsymbol{c}) \times \boldsymbol{p} + \boldsymbol{\tau}. \tag{2.6}$$

2.3. Resultant loads. We suppose that the resultant loads $(\boldsymbol{f}, \boldsymbol{\tau})$ can be decomposed as

$$\boldsymbol{f} = \boldsymbol{f}^{(v)} + \boldsymbol{f}^{(c)} + \boldsymbol{f}^{(s)}, \qquad \boldsymbol{\tau} = \boldsymbol{\tau}^{(v)} + \boldsymbol{\tau}^{(c)} + \boldsymbol{\tau}^{(s)}, \tag{2.7}$$

where $(\boldsymbol{f}^{(v)}, \boldsymbol{\tau}^{(v)})$ denote viscous loads, $(\boldsymbol{f}^{(c)}, \boldsymbol{\tau}^{(c)})$ denote conservative loads, and $(\boldsymbol{f}^{(s)}, \boldsymbol{\tau}^{(s)})$ denote stochastic loads. Here all loads are referred to the reference point $\boldsymbol{r}$. We assume that the viscous loads have a general linear dependence on the linear and angular velocities,

$$\boldsymbol{f}^{(v)} = -\boldsymbol{\gamma}_1 \boldsymbol{v} - \boldsymbol{\gamma}_3 \boldsymbol{\omega}, \qquad \boldsymbol{\tau}^{(v)} = -\boldsymbol{\gamma}_2 \boldsymbol{v} - \boldsymbol{\gamma}_4 \boldsymbol{\omega}, \tag{2.8}$$

where $\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_4$ are given tensors which in general may depend on the configuration of the body. We suppose that the conservative loads $(\boldsymbol{f}^{(c)}, \boldsymbol{\tau}^{(c)})$ satisfy, for all possible motions of the body,

$$\boldsymbol{f}^{(c)} \cdot \boldsymbol{v} + \boldsymbol{\tau}^{(c)} \cdot \boldsymbol{\omega} = -\dot{U}, \tag{2.9}$$

where U is a prescribed potential energy function. Last, we assume that the stochastic loads $(\boldsymbol{f}^{(s)}, \boldsymbol{\tau}^{(s)})$ are white-noise-type loads of the form

$$\boldsymbol{f}^{(s)} = \boldsymbol{\sigma}_1 \dot{\boldsymbol{W}}^{\mathrm{lin}} + \boldsymbol{\sigma}_3 \dot{\boldsymbol{W}}^{\mathrm{ang}}, \qquad \boldsymbol{\tau}^{(s)} = \boldsymbol{\sigma}_2 \dot{\boldsymbol{W}}^{\mathrm{lin}} + \boldsymbol{\sigma}_4 \dot{\boldsymbol{W}}^{\mathrm{ang}}, \tag{2.10}$$

where $\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_4$ are given tensors which in general may depend on the configuration of the body and $(\boldsymbol{W}^{\mathrm{lin}}, \boldsymbol{W}^{\mathrm{ang}})$ denote standard, independent Wiener processes. Following the standard abuse of notation, we represent these loads as derivatives of Wiener processes (which do not exist in any classical sense) rather than in terms of appropriate stochastic integrals.

Remarks 2.1.

1. The form of the viscous loads in (2.8) is consistent with a Stokesian hydrodynamic model of the solvent and is a generalization to a rigid body of arbitrary shape of the classic Stokes laws for the force and torque on a sphere. Detailed discussions of this hydrodynamic model and the hydrodynamic resistance tensors $\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_4$ can be found in [16, 22, 24, 28].
2. The definition of the conservative loads in (2.9) states that the rate of work done by $(\boldsymbol{f}^{(c)}, \boldsymbol{\tau}^{(c)})$ in any motion is equal to the negative rate of change of the potential energy U. This coordinate-free statement is a straightforward generalization to a rigid body of the usual definition of potential loads on a particle.
3. Just as in classic Langevin models, the form of the stochastic loads in (2.10) is motivated by the form of the viscous loads in (2.8). As we will see, when $\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_4$ are related to $\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_4$ through an appropriate fluctuation-dissipation relation [29], the stochastic rigid body model will possess a stationary measure in certain canonical variables.
4. In general, the resultant loads $(\boldsymbol{f}, \boldsymbol{\tau})$ may also contain arbitrary, time-dependent external loads $(\boldsymbol{f}^{(e)}, \boldsymbol{\tau}^{(e)})$. Throughout our developments we shall omit explicit reference to such loads. This is done for simplicity alone; all our results can be generalized in a straightforward way to include them.

2.4. Euler–Langevin equations, components. Substituting (2.7), (2.8), and (2.10) into (2.6), combining the result with (2.4), and using the antisymmetry of the vector product, we obtain the Euler–Langevin equations of motion

$$\begin{aligned}
\dot{\boldsymbol{r}} &= \boldsymbol{v}, \\
\dot{\boldsymbol{d}}_i &= \boldsymbol{\omega} \times \boldsymbol{d}_i, \\
\dot{\boldsymbol{p}} &= \boldsymbol{f}^{(c)} - \boldsymbol{\gamma}_1 \boldsymbol{v} - \boldsymbol{\gamma}_3 \boldsymbol{\omega} + \boldsymbol{\sigma}_1 \dot{\boldsymbol{W}}^{\mathrm{lin}} + \boldsymbol{\sigma}_3 \dot{\boldsymbol{W}}^{\mathrm{ang}}, \\
\dot{\boldsymbol{\pi}} &= \boldsymbol{p} \times (\boldsymbol{c} \times \boldsymbol{\omega}) + \boldsymbol{\tau}^{(c)} - \boldsymbol{\gamma}_2 \boldsymbol{v} - \boldsymbol{\gamma}_4 \boldsymbol{\omega} + \boldsymbol{\sigma}_2 \dot{\boldsymbol{W}}^{\mathrm{lin}} + \boldsymbol{\sigma}_4 \dot{\boldsymbol{W}}^{\mathrm{ang}},
\end{aligned} \tag{2.11}$$

where $\boldsymbol{p} = m(\boldsymbol{v} + \boldsymbol{\omega} \times \boldsymbol{c})$ and $\boldsymbol{\pi} = \boldsymbol{I}\boldsymbol{\omega} + \boldsymbol{c} \times \boldsymbol{p}$. These are vector equations which are defined independently of any choice of reference frame.

We next express (2.11) in terms of a convenient set of components in the frames $\{\boldsymbol{d}_i\}$ and $\{\boldsymbol{e}_i\}$. Let $Q \in SO_3 \subset \mathbb{R}^{3\times 3}$ denote the component matrix of the body frame $\{\boldsymbol{d}_i\}$ in the fixed frame $\{\boldsymbol{e}_i\}$, that is, $Q_{ij} = \boldsymbol{e}_i \cdot \boldsymbol{d}_j$, where SO_3 denotes the set of

proper rotation matrices. Moreover, let $r \in \mathbb{R}^3$, $v \in \mathbb{R}^3$, $\gamma_1 \in \mathbb{R}^{3\times 3}$, and so on denote the component vectors and matrices of all other quantities in the frame $\{\boldsymbol{d}_i\}$, that is, $r_i = \boldsymbol{d}_i \cdot \boldsymbol{r}$, $v_i = \boldsymbol{d}_i \cdot \boldsymbol{v}$, $\gamma_1^{ij} = \boldsymbol{d}_i \cdot \boldsymbol{\gamma}_1 \boldsymbol{d}_j$, and so on. Then by straightforward calculation we find that the equations in (2.11) become

$$\begin{aligned} \dot{r} &= r \times \omega + v, \\ \dot{Q} &= Q[\omega\times], \\ \dot{p} &= p \times \omega + f^{(c)} - \gamma_1 v - \gamma_3 \omega + \sigma_1 \dot{W}^{\mathrm{lin}} + \sigma_3 \dot{W}^{\mathrm{ang}}, \\ \dot{\pi} &= \pi \times \omega + p \times (c \times \omega) + \tau^{(c)} - \gamma_2 v - \gamma_4 \omega + \sigma_2 \dot{W}^{\mathrm{lin}} + \sigma_4 \dot{W}^{\mathrm{ang}}, \end{aligned} \tag{2.12}$$

where $p = m(v + \omega \times c)$, $\pi = I\omega + c \times p$, and $[\omega\times] \in \mathbb{R}^{3\times 3}$ denotes the skew-symmetric matrix

$$[\omega\times] = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}. \tag{2.13}$$

By definition, this matrix has the property that $[\omega\times]g = \omega \times g$ for all component vectors g. Moreover, we have $[\omega\times]_{ij} = \epsilon_{ikj}\omega_k$, where ϵ_{ikj} is the standard permutation symbol of vector analysis. Here and throughout we use the usual summation convention on pairs of repeated indices. To derive (2.12) we made use of the identity $A(a \times b) = Aa \times Ab$, which holds for any proper rotation matrix $A \in SO_3$ and vectors $a, b \in \mathbb{R}^3$.

We interpret (2.12) as a system of stochastic differential equations in the sense of Itô for the phase variables (r, Q, p, π) which evolve in the space $\mathbb{R}^3 \times SO_3 \times \mathbb{R}^3 \times \mathbb{R}^3$. In this system, the scalar m, the component vector c, and the component matrix I are all assumed to be constant. The component matrices $\gamma_1, \ldots, \gamma_4$ and $\sigma_1, \ldots, \sigma_4$ and the function U appearing in (2.8), (2.9), and (2.10) are all assumed to be functions of the configuration variables (r, Q). Notice that, in terms of components, those equations become

$$\begin{gathered} f^{(v)} = -\gamma_1 v - \gamma_3 \omega, \qquad \tau^{(v)} = -\gamma_2 v - \gamma_4 \omega, \\ f^{(c)} \cdot v + \tau^{(c)} \cdot \omega = -\dot{U}, \\ f^{(s)} = \sigma_1 \dot{W}^{\mathrm{lin}} + \sigma_3 \dot{W}^{\mathrm{ang}}, \qquad \tau^{(s)} = \sigma_2 \dot{W}^{\mathrm{lin}} + \sigma_4 \dot{W}^{\mathrm{ang}}. \end{gathered} \tag{2.14}$$

Remarks 2.2.

1. We assume that the component matrices $\gamma_1, \ldots, \gamma_4$ and $\sigma_1, \ldots, \sigma_4$ and the function U are all smooth functions of the configuration variables $(r, Q) \in \mathbb{R}^3 \times SO_3$. Moreover, when working in local coordinates for SO_3, we will assume that the coordinate chart as well as its associated inverse chart are smooth. Furthermore, we will assume that all changes of variables as well as their inverses are smooth. These assumptions are stronger than necessary, but they allow for a clean presentation of our results.
2. Our choice to work with body-frame components in (2.12) is motivated by the fact that, by definition, the inertia matrix I is constant in this frame, which will simplify our developments. In many applications, the resistance matrices $\gamma_1, \ldots, \gamma_4$ are also constant in this frame [16, 22, 28]; however, we make no assumption along these lines. In view of Propositions 3.7 and 3.9 below, there is no loss of generality in this choice of frame.
3. In general, for a system of stochastic equations with multiplicative noise as in (2.12), there is a distinction between their Itô and Stratonovich interpretations [41]. Here, however, it can be shown that this distinction vanishes

due to the fact that the noise terms appear only in the momentum equations and that they have coefficients that depend only on the configuration variables. In contrast, it can be shown that the distinction becomes relevant in the high-friction limit of (2.12).

4. An important property of the formulation in (2.12) is the allowed coupling between translational and rotational motions. If this coupling is assumed to vanish, then translational and rotational motions can be studied independently. The equations for translational motion in the decoupled case (which are most naturally expressed using components in a fixed frame) reduce to that of a particle and are covered by the classic theory [8, 18, 45]. The equations for rotational motion are less well studied; various results for different models can be found in [34, 39].
5. Existence and uniqueness of solutions to general systems of stochastic differential equations are guaranteed by classic theory when the coefficient functions satisfy suitable Lipschitz and growth conditions [2, 17]. While a detailed analysis of such issues for (2.12) is beyond the scope of this article, we remark that various results have been established for related systems under various different assumptions [25, 36, 37, 50]. Throughout we shall assume that, for any given initial condition, the system in (2.12) has a unique solution defined for all positive time.

3. Hamiltonian formulations. Here we discuss local coordinates for SO_3 and use the change of variables formula of Itô [41] to show that the equations of motion in (2.12) can be put into both canonical and noncanonical Hamiltonian–Langevin forms. Moreover, we show that these forms are invariant under an arbitrary change of configuration variables. Similar results for particle systems can be found in [7, 23, 27].

3.1. Local coordinates for SO_3. Consider an arbitrary coordinate chart $Q = Q(\eta) : \mathcal{A} \to \mathcal{R}$, with inverse $\eta = \eta(Q) : \mathcal{R} \to \mathcal{A}$, where $\mathcal{A} \subset \mathbb{R}^3$ and $\mathcal{R} \subset SO_3$ are open subsets. Given any such chart, we consider an associated matrix $S = S(\eta) : \mathcal{A} \to \mathbb{R}^{3\times 3}$, which we call the angular velocity structure matrix, defined by

$$S_{mj} = \frac{1}{2}\epsilon_{imk} Q_{li} \frac{\partial Q_{lk}}{\partial \eta_j} = \frac{1}{2}\epsilon_{imk}\left[Q^T \frac{\partial Q}{\partial \eta_j}\right]_{ik}. \tag{3.1}$$

Consistent with the invertibility of the chart, we assume that $S \in \mathbb{R}^{3\times 3}$ is invertible for all $\eta \in \mathcal{A}$. Indeed, as shown below, differential three-volume elements in $\mathcal{R}$ and $\mathcal{A}$ are related as $dQ = g d\eta$, where $g = 2^{3/2}|S|$ is the associated Jacobian determinant factor. For simplicity, we assume that $\mathcal{R}$ has full measure in SO_3, which will allow us to state all results in terms of a single chart rather than an atlas of overlapping charts. Without loss of generality, we assume that $\mathcal{A}$ is the Cartesian product of possibly unbounded open intervals $\mathcal{A}_i$, where each coordinate η_i is either regular or singular in the sense that $|S| \neq 0$ or $|S| = 0$ on $\partial\mathcal{A}_i$ (points at infinity included). Furthermore, we assume that the local representation of any function on SO_3 is periodic in the regular coordinates. For convenience, we will use the more descriptive terms cyclic and acyclic in place of regular and singular, respectively, and will assume that any cyclic coordinates are bounded.

Various different standard coordinate charts satisfy the above assumptions. All the various different Euler angle charts [26] provide one family of examples, each of which has a bounded coordinate domain $\mathcal{A} \subset \mathbb{R}^3$ and one acyclic and two cyclic coordinates. The Cayley (also referred to as Euler–Rodrigues or Gibbs) chart [26] and

its variations provide another family of examples, each of which has an unbounded coordinate domain $\mathcal{A} = \mathbb{R}^3$ and three acyclic coordinates, with coordinates at infinity representing rotations through π-radians. Charts based on Euler coordinates would be natural for the modeling of bodies with unrestrained rotational degrees of freedom, whereas charts based on Cayley coordinates would be natural for the modeling of bodies with strongly restrained rotational degrees of freedom, for example, bodies whose relative rotations about any axis are inherently restricted to be through an angle less than π.

Our first result, which involves only deterministic calculus on SO_3, establishes an important connection between the structure matrix S and the derivatives of Q, a certain commutation identity for the derivatives of S, and a relation between the volume elements dQ and $d\eta$.

PROPOSITION 3.1. *The structure matrix S and volume elements dQ and $d\eta$ satisfy*

(i) $\frac{d}{d\alpha}Q(\eta+\alpha a)\big|_{\alpha=0} = Q[(Sa)\times]$ *or* $\frac{\partial Q_{ij}}{\partial \eta_k}a_k = Q_{in}[(Sa)\times]_{nj}$ *for all* $a \in \mathbb{R}^3$,

(ii) $\frac{\partial S_{mj}}{\partial \eta_r} - \frac{\partial S_{mr}}{\partial \eta_j} = \frac{1}{2}\epsilon_{imk}\big(S_{kj}S_{ir} - S_{kr}S_{ij}\big)$,

(iii) $dQ = 2^{3/2}|S|\, d\eta$.

Proof. To establish (i) let a be arbitrary and consider the curve $Q(\eta+\alpha a) \in SO_3$ defined for all $\alpha \in \mathbb{R}$ sufficiently small. Differentiating the orthogonality relation $Q^TQ = \mathrm{Id}$ with respect to α at $\alpha = 0$, where $\mathrm{Id} \in \mathbb{R}^{3\times 3}$ denotes the identity matrix, we get $[Q']^TQ + Q^TQ' = 0$, which implies

$$Q^TQ' = -[Q^TQ']^T. \tag{3.2}$$

By the definition of S in (3.1) and the chain rule, we have

$$S_{mj}a_j = \tfrac{1}{2}\epsilon_{imk}Q_{li}\tfrac{\partial Q_{lk}}{\partial \eta_j}a_j = \tfrac{1}{2}\epsilon_{imk}Q_{li}Q'_{lk} = \tfrac{1}{2}\epsilon_{imk}[Q^TQ']_{ik}. \tag{3.3}$$

Multiplying the above result by ϵ_{pmq}, summing over m, and using the well-known tensor analysis identity $\epsilon_{pmq}\epsilon_{imk} = \delta_{pi}\delta_{qk} - \delta_{pk}\delta_{qi}$, where δ_{ij} is the Kronecker delta symbol, we get

$$\epsilon_{pmq}S_{mj}a_j = \tfrac{1}{2}(\delta_{pi}\delta_{qk} - \delta_{pk}\delta_{qi})[Q^TQ']_{ik} = \tfrac{1}{2}([Q^TQ']_{pq} - [Q^TQ']_{qp}). \tag{3.4}$$

Using (2.13), we can express the above result in the matrix form

$$[(Sa)\times] = \tfrac{1}{2}(Q^TQ' - [Q^TQ']^T) = Q^TQ', \tag{3.5}$$

where the last equality follows from (3.2). Multiplying both sides by Q yields the desired result.

To establish (ii) we differentiate the relation in (3.1) with respect to η_r and obtain

$$\frac{\partial S_{mj}}{\partial \eta_r} = \frac{1}{2}\epsilon_{imk}\left[\frac{\partial Q^T}{\partial \eta_r}\frac{\partial Q}{\partial \eta_j}\right]_{ik} + \frac{1}{2}\epsilon_{imk}\left[Q^T\frac{\partial^2 Q}{\partial \eta_j \partial \eta_r}\right]_{ik}. \tag{3.6}$$

Using the orthogonality of Q, we can rewrite the first term in brackets on the right-hand side of the above equation as

$$\left[\frac{\partial Q^T}{\partial \eta_r}\frac{\partial Q}{\partial \eta_j}\right]_{ik} = \left[\left(Q^T\frac{\partial Q}{\partial \eta_r}\right)^T\left(Q^T\frac{\partial Q}{\partial \eta_j}\right)\right]_{ik} = \left[Q^T\frac{\partial Q}{\partial \eta_r}\right]_{li}\left[Q^T\frac{\partial Q}{\partial \eta_j}\right]_{lk}. \tag{3.7}$$

Moreover, from (2.13) and part (i) with $a = e_j$, where $e_j \in \mathbb{R}^3$ denotes the jth standard unit vector, we have

$$\left[Q^T \frac{\partial Q}{\partial \eta_j}\right]_{pq} = \epsilon_{pmq} S_{mj}. \tag{3.8}$$

Using (3.8) in (3.7) and substituting the result into (3.6), we get

$$\frac{\partial S_{mj}}{\partial \eta_r} = \frac{1}{2}\epsilon_{imk}\epsilon_{lni}\epsilon_{lpk} S_{nr} S_{pj} + \frac{1}{2}\epsilon_{imk}\left[Q^T \frac{\partial^2 Q}{\partial \eta_j \partial \eta_r}\right]_{ik}. \tag{3.9}$$

Furthermore, using the identity $\epsilon_{lni}\epsilon_{lpk} = \delta_{np}\delta_{ik} - \delta_{nk}\delta_{ip}$, together with the fact that $\epsilon_{imk}\delta_{ik} = 0$, we obtain

$$\frac{\partial S_{mj}}{\partial \eta_r} = -\frac{1}{2}\epsilon_{imk} S_{kr} S_{ij} + \frac{1}{2}\epsilon_{imk}\left[Q^T \frac{\partial^2 Q}{\partial \eta_j \partial \eta_r}\right]_{ik}, \tag{3.10}$$

and interchanging the indices j and r we find

$$\frac{\partial S_{mr}}{\partial \eta_j} = -\frac{1}{2}\epsilon_{imk} S_{kj} S_{ir} + \frac{1}{2}\epsilon_{imk}\left[Q^T \frac{\partial^2 Q}{\partial \eta_r \partial \eta_j}\right]_{ik}. \tag{3.11}$$

The desired result now follows by subtracting (3.11) from (3.10) and noting that the second-order mixed partial derivatives of Q are equal.

To establish (iii) we consider SO_3 as a manifold in $\mathbb{R}^{3\times 3} = \mathbb{R}^9$ parameterized by a chart $Q(\eta)$ with Jacobian matrix $DQ(\eta) \in \mathbb{R}^{9\times 3}$. In terms of a chart, the intrinsic three-volume of any open subset $\mathcal{O} \subset \mathcal{R}$ with preimage $Q^{-1}(\mathcal{O}) \subset \mathcal{A}$ is given by [40, 51]

$$\mathrm{vol}(\mathcal{O}) = \int_{\mathcal{O}} dQ = \int_{Q^{-1}(\mathcal{O})} g\, d\eta, \qquad g = \sqrt{|DQ^T DQ|}. \tag{3.12}$$

The matrix $DQ^T DQ \in \mathbb{R}^{3\times 3}$ can be expressed in terms of S. Indeed, using the orthogonality of Q, part (i) with $a = e_k$ and $a = e_l$, and the definition of the skew-symmetric matrix in (2.13), we have

$$\begin{aligned}
[DQ^T DQ]_{kl} = \frac{\partial Q_{ij}}{\partial \eta_k}\frac{\partial Q_{ij}}{\partial \eta_l} &= Q_{nr}\frac{\partial Q_{nj}}{\partial \eta_k} Q_{mr}\frac{\partial Q_{mj}}{\partial \eta_l} \\
&= \left[Q^T \frac{\partial Q}{\partial \eta_k}\right]_{rj}\left[Q^T \frac{\partial Q}{\partial \eta_l}\right]_{rj} \\
&= \Big[(Se_k)\times\Big]_{rj}\Big[(Se_l)\times\Big]_{rj} \\
&= 2(Se_k)\cdot(Se_l) = 2[S^T S]_{kl}.
\end{aligned} \tag{3.13}$$

From this we deduce that $DQ^T DQ = 2S^T S$, and the result follows. ∎

The next result shows that if $(r, Q, p, \pi)(t)$ is any process satisfying the equations in (2.12), then the process $\eta(t)$ satisfies a particularly simple equation with no diffusion.

PROPOSITION 3.2. *Let $(r, Q, p, \pi)(t)$ be any process satisfying the equations in (2.12). Then the process $\eta(t)$ satisfies the equation*

$$\dot{\eta} = S^{-1}\omega, \tag{3.14}$$

where $S = S(\eta)$ is the associated angular velocity structure matrix and $\omega = I^{-1}(\pi - c \times p)$ is the body angular velocity.

Proof. The fact that $Q(t)$ is an Itô process implies that $\eta(t) = \eta(Q(t))$ is also an Itô process, which in general can be characterized by an equation of the form

$$\mathsf{d}\eta = A(\eta, t)\mathsf{d}t + B(\eta, t)\mathsf{d}W \tag{3.15}$$

for some coefficient functions $A(\eta, t) \in \mathbb{R}^3$ and $B(\eta, t) \in \mathbb{R}^{3\times 3}$, where $W(t) \in \mathbb{R}^3$ denotes a standard Wiener process and d denotes a differential increment. To determine $A(\eta, t)$ and $B(\eta, t)$, let $\eta(t)$ satisfy (3.15) and consider $Q(\eta(t))$. Then, by Itô's formula, we have

$$\mathsf{d}[Q(\eta)]_{ij} = \frac{\partial Q_{ij}}{\partial \eta_k}\mathsf{d}\eta_k + \frac{1}{2}\frac{\partial^2 Q_{ij}}{\partial \eta_k \partial \eta_l}\mathsf{d}\eta_k \mathsf{d}\eta_l. \tag{3.16}$$

Substituting (3.15) into (3.16) and omitting the arguments of A and B for clarity, we get

$$\begin{aligned} \mathsf{d}[Q(\eta)]_{ij} &= \frac{\partial Q_{ij}}{\partial \eta_k}\Big[A_k \mathsf{d}t + B_{kn}\mathsf{d}W_n\Big] \\ &\quad + \frac{1}{2}\frac{\partial^2 Q_{ij}}{\partial \eta_k \partial \eta_l}\Big[A_k \mathsf{d}t + B_{kn}\mathsf{d}W_n\Big]\Big[A_l \mathsf{d}t + B_{lm}\mathsf{d}W_m\Big]. \end{aligned} \tag{3.17}$$

Using the stochastic calculus rules $\mathsf{d}t\mathsf{d}t = 0$, $\mathsf{d}t\mathsf{d}W_i = 0$, and $\mathsf{d}W_i\mathsf{d}W_j = \delta_{ij}\,\mathsf{d}t$, we obtain

$$\mathsf{d}[Q(\eta)]_{ij} = \left[\frac{\partial Q_{ij}}{\partial \eta_k}A_k + \frac{1}{2}\frac{\partial^2 Q_{ij}}{\partial \eta_k \partial \eta_l}B_{kn}B_{ln}\right]\mathsf{d}t + \frac{\partial Q_{ij}}{\partial \eta_k}B_{kn}\mathsf{d}W_n. \tag{3.18}$$

Alternatively, from (2.12) we have

$$\mathsf{d}Q_{ij} = Q_{ip}[\omega\times]_{pj}\,\mathsf{d}t. \tag{3.19}$$

Comparing (3.19) and (3.18) we deduce that the diffusion term in (3.18) must vanish. By Proposition 3.1(i), this term can be written in the form

$$\frac{\partial Q_{ij}}{\partial \eta_k}B_{kn}\mathsf{d}W_n = Q_{ip}[(SB\mathsf{d}W)\times]_{pj}. \tag{3.20}$$

Since Q is invertible, the diffusion term vanishes if and only if $[(SB\mathsf{d}W)\times]$ vanishes. Moreover, since S is invertible, $[(SB\mathsf{d}W)\times]$ vanishes if and only if $B\mathsf{d}W$ vanishes. Thus we conclude that B must vanish. Setting $B = 0$ in (3.15) and (3.18) and combining the resulting equations, we find

$$\mathsf{d}[Q(\eta)]_{ij} = \frac{\partial Q_{ij}}{\partial \eta_k}\mathsf{d}\eta_k = Q_{ip}[(S\mathsf{d}\eta)\times]_{pj}, \tag{3.21}$$

where the last equality follows from Proposition 3.1(i). From (3.21), (3.19), and (2.13) we then deduce that

$$S\mathsf{d}\eta = \omega\mathsf{d}t, \tag{3.22}$$

which yields the desired result. ∎

3.2. Velocity structure matrix, kinetic energy, momenta. Consider the configuration variables (r, η), where η are any local coordinates for SO_3. From $(2.12)_1$ and (3.14) we find that the velocity components (v, ω) can be expressed as a function of $(r, \eta, \dot{r}, \dot{\eta})$, that is,

$$\begin{pmatrix} v \\ \omega \end{pmatrix} = \begin{pmatrix} \dot{r} - r \times \omega \\ S\dot{\eta} \end{pmatrix} = G \begin{pmatrix} \dot{r} \\ \dot{\eta} \end{pmatrix}, \tag{3.23}$$

where $G = G(r, \eta) \in \mathbb{R}^{6\times 6}$ is an invertible matrix depending on the choice of coordinates for SO_3, namely

$$G = \begin{pmatrix} \mathrm{Id} & -[r\times]S \\ 0 & S \end{pmatrix}, \qquad G^{-1} = \begin{pmatrix} \mathrm{Id} & [r\times] \\ 0 & S^{-1} \end{pmatrix}. \tag{3.24}$$

Here and in the following, Id denotes the identity matrix whose dimension is set by the context. Notice that the invertibility of G may not be uniform since the determinant $|G| = |S|$ vanishes at the limiting boundary values of any acyclic rotational coordinates. We will refer to G as the velocity structure matrix associated with the configuration variables (r, η); it will play an important role throughout our developments.

The kinetic energy of the body is a function $\Phi(v, \omega)$ defined by

$$\Phi(v, \omega) = \tfrac{1}{2}(v + \omega \times c) \cdot m(v + \omega \times c) + \tfrac{1}{2}\omega \cdot I\omega, \tag{3.25}$$

where $v + \omega \times c$ is the velocity of the center of mass. By expanding the first term on the right-hand side of (3.25), we find that $\Phi(v, \omega)$ can be written in the convenient form

$$\Phi(v, \omega) = \frac{1}{2} \begin{pmatrix} v \\ \omega \end{pmatrix} \cdot M \begin{pmatrix} v \\ \omega \end{pmatrix}, \tag{3.26}$$

where $M \in \mathbb{R}^{6\times 6}$ is a constant, symmetric, positive-definite generalized mass matrix given, along with its inverse, by

$$\begin{aligned} M &= \begin{pmatrix} m\mathrm{Id} & m[c\times]^T \\ m[c\times] & I + m[c\times][c\times]^T \end{pmatrix}, \\ M^{-1} &= \begin{pmatrix} m^{-1}\mathrm{Id} + [c\times]I^{-1}[c\times]^T & [c\times]I^{-1} \\ I^{-1}[c\times]^T & I^{-1} \end{pmatrix}. \end{aligned} \tag{3.27}$$

The equations of motion can be formulated in terms of different momentum variables [19, 26]. In their most basic form as in (2.12), they are formulated in terms of (p, π), which are given by

$$\begin{pmatrix} p \\ \pi \end{pmatrix} = \begin{pmatrix} m(v + \omega \times c) \\ c \times p + I\omega \end{pmatrix} = M \begin{pmatrix} v \\ \omega \end{pmatrix}. \tag{3.28}$$

Alternatively, the equations of motion can be put into a certain canonical form by introducing momentum variables (ψ, ζ) associated with (r, η), namely

$$\psi = \frac{\partial T}{\partial \dot{r}}, \qquad \zeta = \frac{\partial T}{\partial \dot{\eta}}, \tag{3.29}$$

where T is the kinetic energy of the body expressed as a function of $(r, \eta, \dot{r}, \dot{\eta})$. Specifically, using (3.26) and (3.23), we have

$$T(r,\eta,\dot{r},\dot{\eta}) = \Phi(v,\omega)\Big|_{\substack{v=v(r,\eta,\dot{r},\dot{\eta})\\ \omega=\omega(r,\eta,\dot{r},\dot{\eta})}} = \frac{1}{2}\begin{pmatrix} \dot{r} \\ \dot{\eta} \end{pmatrix} \cdot G^T M G \begin{pmatrix} \dot{r} \\ \dot{\eta} \end{pmatrix}. \tag{3.30}$$

The variables (ψ, ζ) are called the canonical or conjugate momenta associated with (r, η). From (3.29) and (3.30) we deduce that

$$\begin{pmatrix} \psi \\ \zeta \end{pmatrix} = G^T M G \begin{pmatrix} \dot{r} \\ \dot{\eta} \end{pmatrix}. \tag{3.31}$$

Various relations between (v, ω), (p, π), and (ψ, ζ) can be deduced from (3.23), (3.28), and (3.31). The relations that will be most useful for our developments are

$$\begin{gathered} \begin{pmatrix} v \\ \omega \end{pmatrix} = M^{-1}\begin{pmatrix} p \\ \pi \end{pmatrix}, \qquad \begin{pmatrix} v \\ \omega \end{pmatrix} = M^{-1}G^{-T}\begin{pmatrix} \psi \\ \zeta \end{pmatrix}, \\ \begin{pmatrix} \psi \\ \zeta \end{pmatrix} = G^T \begin{pmatrix} p \\ \pi \end{pmatrix}. \end{gathered} \tag{3.32}$$

Carrying out the matrix products in each of the three relations in (3.32), we find

$$\begin{gathered} v = m^{-1}p + c \times \omega, \qquad \omega = I^{-1}\big(\pi - c \times p\big), \\ v = m^{-1}\psi + c \times \omega, \qquad \omega = I^{-1}\big(S^{-T}\zeta - (r+c) \times \psi\big), \\ \psi = p, \qquad \zeta = S^T\big(\pi + r \times p\big). \end{gathered} \tag{3.33}$$

In reformulating the equations of motion it will be useful to express the kinetic energy in terms of different sets of variables. In terms of the noncanonical variables (r, η, p, π) we have

$$\Upsilon(r,\eta,p,\pi) = \Phi(v,\omega)\Big|_{\substack{v=v(r,\eta,p,\pi)\\ \omega=\omega(r,\eta,p,\pi)}} = \frac{1}{2}\begin{pmatrix} p \\ \pi \end{pmatrix} \cdot M^{-1} \begin{pmatrix} p \\ \pi \end{pmatrix}. \tag{3.34}$$

Here we consider (v, ω) as functions of (r, η, p, π) via the first equation in (3.32), or equivalently the first pair of equations in (3.33). Similarly, in terms of the canonical variables (r, η, ψ, ζ) we have

$$\Psi(r,\eta,\psi,\zeta) = \Phi(v,\omega)\Big|_{\substack{v=v(r,\eta,\psi,\zeta)\\ \omega=\omega(r,\eta,\psi,\zeta)}} = \frac{1}{2}\begin{pmatrix} \psi \\ \zeta \end{pmatrix} \cdot G^{-1}M^{-1}G^{-T} \begin{pmatrix} \psi \\ \zeta \end{pmatrix}. \tag{3.35}$$

Here we consider (v, ω) as functions of (r, η, ψ, ζ) via the second equation in (3.32), or equivalently the second pair of equations in (3.33).

The following result provides explicit expressions for the partial derivatives of Υ and Ψ, which will be useful in establishing various Hamiltonian formulations of (2.12).

PROPOSITION 3.3. *Let $\Upsilon(r, \eta, p, \pi)$ and $\Psi(r, \eta, \psi, \zeta)$ be the functions defined in* (3.34) *and* (3.35). *Then*

$$\begin{gathered} \frac{\partial \Upsilon}{\partial p} = v, \qquad \frac{\partial \Upsilon}{\partial \pi} = \omega, \qquad \frac{\partial \Upsilon}{\partial r} = 0, \qquad \frac{\partial \Upsilon}{\partial \eta} = 0, \\ \frac{\partial \Psi}{\partial \psi} = r \times \omega + v, \qquad \frac{\partial \Psi}{\partial \zeta} = S^{-1}\omega, \qquad \frac{\partial \Psi}{\partial r} = -p \times \omega, \\ \frac{\partial \Psi}{\partial \eta_l} = -\frac{\partial S_{ml}}{\partial \eta_j}\Big[S^{-1}\omega\Big]_j\Big[\pi + r \times p\Big]_m - \Big[S^T\Big(\pi \times \omega + (r \times p) \times \omega\Big)\Big]_l. \end{gathered} \tag{3.36}$$

Proof. All of the partials of Υ, and those of Ψ with respect to ψ, ζ, and r, follow from straightforward applications of the chain rule. To establish the result for Ψ with respect to η, we use (3.35) and the second pair of relations in (3.33) to write

$$\frac{\partial \Psi}{\partial \eta_l} = \left(\frac{\partial \Phi}{\partial v_k} \frac{\partial v_k}{\partial \omega_i} + \frac{\partial \Phi}{\partial \omega_i} \right) \frac{\partial \omega_i}{\partial \eta_l} = \left[\left(\frac{\partial v}{\partial \omega} \right)^T \frac{\partial \Phi}{\partial v} + \frac{\partial \Phi}{\partial \omega} \right]_i \left[\frac{\partial \omega}{\partial \eta_l} \right]_i . \tag{3.37}$$

From the second pair of relations in (3.33) we find $\partial v/\partial \omega = [c\times]$ and $\partial \omega/\partial \eta_l = I^{-1}(\frac{\partial}{\partial \eta_l} S^{-1})^T \zeta$, and from (3.26) and (3.28) we find $\partial \Phi/\partial v = p$ and $\partial \Phi/\partial \omega = \pi$. Substituting these results into (3.37) we get

$$\frac{\partial \Psi}{\partial \eta_l} = \Big[\pi - c \times p \Big]_i \left[\frac{\partial \omega}{\partial \eta_l} \right]_i = \Big[I\omega \Big]_i \left[I^{-1} \left(\frac{\partial}{\partial \eta_l} S^{-1} \right)^T \zeta \right]_i , \tag{3.38}$$

where the last equality follows upon substituting for $\pi - c \times p$ from (3.33).

Using the fact that $(A^{-1})' = -A^{-1} A' A^{-1}$ for any invertible matrix $A(\alpha)$, $\alpha \in \mathbb{R}$, we get

$$\frac{\partial \Psi}{\partial \eta_l} = -\Big[I\omega \Big]_i \left[I^{-1} S^{-T} \left(\frac{\partial S}{\partial \eta_l} \right)^T S^{-T} \zeta \right]_i . \tag{3.39}$$

Writing the above relation as a dot product and using properties of the matrix transpose and the symmetry of I, we obtain

$$\frac{\partial \Psi}{\partial \eta_l} = -I\omega \cdot I^{-1} S^{-T} \left(\frac{\partial S}{\partial \eta_l} \right)^T S^{-T} \zeta = -\frac{\partial S}{\partial \eta_l} S^{-1} \omega \cdot S^{-T} \zeta . \tag{3.40}$$

Using components, we can write the above relation in the form

$$\frac{\partial \Psi}{\partial \eta_l} = -\frac{\partial S_{mj}}{\partial \eta_l} \Big[S^{-1} \omega \Big]_j \Big[S^{-T} \zeta \Big]_m . \tag{3.41}$$

Substituting for $\partial S_{mj}/\partial \eta_l$ from Proposition 3.1(ii) and using the notation $b = S^{-T}\zeta$ and properties of matrix multiplication, we get

$$\begin{aligned} \tfrac{\partial \Psi}{\partial \eta_l} &= -\Big(\tfrac{\partial S_{ml}}{\partial \eta_j} + \tfrac{1}{2} \epsilon_{imk} S_{kj} S_{il} - \tfrac{1}{2} \epsilon_{imk} S_{kl} S_{ij} \Big) \Big[S^{-1} \omega \Big]_j b_m \\ &= -\tfrac{\partial S_{ml}}{\partial \eta_j} \Big[S^{-1} \omega \Big]_j b_m - \tfrac{1}{2} \epsilon_{imk} S_{il} \omega_k b_m + \tfrac{1}{2} \epsilon_{imk} S_{kl} \omega_i b_m \\ &= -\tfrac{\partial S_{ml}}{\partial \eta_j} \Big[S^{-1} \omega \Big]_j b_m - \tfrac{1}{2} S_{il} \Big[b \times \omega \Big]_i + \tfrac{1}{2} S_{kl} \Big[\omega \times b \Big]_k , \end{aligned} \tag{3.42}$$

where the last line follows from the representation of the vector product using (2.13). Simplifying using the antisymmetry of the vector product and properties of matrix multiplication, we obtain

$$\frac{\partial \Psi}{\partial \eta_l} = -\frac{\partial S_{ml}}{\partial \eta_j} \Big[S^{-1} \omega \Big]_j b_m - \Big[S^T \big(b \times \omega \big) \Big]_l . \tag{3.43}$$

By definition, we have $b = S^{-T}\zeta$, and from (3.33) we have $S^{-T}\zeta = \pi + r \times p$. Substituting these relations into (3.43) we get

$$\frac{\partial \Psi}{\partial \eta_l} = -\frac{\partial S_{ml}}{\partial \eta_j} \Big[S^{-1} \omega \Big]_j \Big[\pi + r \times p \Big]_m - \Big[S^T \Big(\pi \times \omega + (r \times p) \times \omega \Big) \Big]_l , \tag{3.44}$$

which is the desired result. ∎

3.3. Resultant loads. Here we establish some convenient expressions for the components $(f^{(v)}, \tau^{(v)})$, $(f^{(c)}, \tau^{(c)})$, and $(f^{(s)}, \tau^{(s)})$ given in (2.14). Our first result provides an explicit characterization of the conservative load components $(f^{(c)}, \tau^{(c)})$ in terms of the derivatives of the potential energy U with respect to the configuration variables (r, η), where η are any local coordinates for SO_3.

PROPOSITION 3.4. *For all possible processes* $(r, \eta)(t)$ *consistent with* (2.12) *and* (3.14) *let* $(f^{(c)}, \tau^{(c)})$ *satisfy*

$$f^{(c)} \cdot v + \tau^{(c)} \cdot \omega = -\dot{U}, \tag{3.45}$$

where $U = U(r, \eta)$ *is a given potential energy function. Then*

$$f^{(c)} = -\frac{\partial U}{\partial r}, \qquad \tau^{(c)} = r \times \frac{\partial U}{\partial r} - S^{-T}\frac{\partial U}{\partial \eta}, \tag{3.46}$$

or in matrix form

$$\begin{pmatrix} f^{(c)} \\ \tau^{(c)} \end{pmatrix} = -G^{-T} \begin{pmatrix} \frac{\partial U}{\partial r} \\ \frac{\partial U}{\partial \eta} \end{pmatrix}. \tag{3.47}$$

Proof. Applying Itô's formula to the function $U(r, \eta)$ and using the fact that $(2.12)_1$ and (3.14) for r and η contain no diffusion terms, we find

$$\mathsf{d}[U(r, \eta)] = \frac{\partial U}{\partial r_k}\mathsf{d}r_k + \frac{\partial U}{\partial \eta_k}\mathsf{d}\eta_k, \tag{3.48}$$

which, using matrix notation, implies

$$\dot{U}(r, \eta) = \frac{\partial U}{\partial r} \cdot \dot{r} + \frac{\partial U}{\partial \eta} \cdot \dot{\eta}. \tag{3.49}$$

Substituting this result into (3.45) and using the relations $v = \dot{r} + \omega \times r$ and $\omega = S\dot{\eta}$, the identity $(x \times y) \cdot z = x \cdot (y \times z)$, and properties of the matrix transpose, we get

$$f^{(c)} \cdot \dot{r} + S^T\big(\tau^{(c)} + r \times f^{(c)}\big) \cdot \dot{\eta} = -\frac{\partial U}{\partial r} \cdot \dot{r} - \frac{\partial U}{\partial \eta} \cdot \dot{\eta}. \tag{3.50}$$

The desired result then follows from the arbitrariness of $\dot{r}$ and $\dot{\eta}$. For this last step, notice that (3.45) is assumed to hold for all possible processes, and moreover, with suitable time-dependent external loads, which can be determined using (2.12) and (3.14), a process with any given values of $\dot{r}$ and $\dot{\eta}$ can be achieved. ∎

We next consider the viscous and stochastic load components $(f^{(v)}, \tau^{(v)})$ and $(f^{(s)}, \tau^{(s)})$. Let $\gamma = \gamma(r, \eta) \in \mathbb{R}^{6\times 6}$, $\sigma = \sigma(r, \eta) \in \mathbb{R}^{6\times 6}$, and $W \in \mathbb{R}^6$ be given, in block form, by

$$\gamma = \begin{pmatrix} \gamma_1 & \gamma_3 \\ \gamma_2 & \gamma_4 \end{pmatrix}, \qquad \sigma = \begin{pmatrix} \sigma_1 & \sigma_3 \\ \sigma_2 & \sigma_4 \end{pmatrix}, \qquad W = \begin{pmatrix} W^{\text{lin}} \\ W^{\text{ang}} \end{pmatrix}. \tag{3.51}$$

The proof of the following result is a straightforward consequence of (2.14) and Proposition 3.3 and is omitted for brevity.

PROPOSITION 3.5. *The components* $(f^{(v)}, \tau^{(v)})$ *and* $(f^{(s)}, \tau^{(s)})$ *can be written in the form*

$$\begin{pmatrix} f^{(v)} \\ \tau^{(v)} \end{pmatrix} = -\gamma \begin{pmatrix} \frac{\partial \Upsilon}{\partial p} \\ \frac{\partial \Upsilon}{\partial \pi} \end{pmatrix} = -\gamma G \begin{pmatrix} \frac{\partial \Psi}{\partial \psi} \\ \frac{\partial \Psi}{\partial \zeta} \end{pmatrix}, \qquad \begin{pmatrix} f^{(s)} \\ \tau^{(s)} \end{pmatrix} = \sigma \dot{W}. \tag{3.52}$$

3.4. Canonical Hamilton–Langevin formulation. Consider the configuration variables (r, η) with associated conjugate momenta variables (ψ, ζ) and the Hamiltonian function defined by

$$H(r, \eta, \psi, \zeta) = \Psi(r, \eta, \psi, \zeta) + U(r, \eta), \tag{3.53}$$

where $\Psi(r, \eta, \psi, \zeta)$ and $U(r, \eta)$ are the kinetic and potential energy functions. Let $J \in \mathbb{R}^{12\times 12}$, $\Gamma = \Gamma(r, \eta) \in \mathbb{R}^{12\times 12}$, and $\Sigma = \Sigma(r, \eta) \in \mathbb{R}^{12\times 6}$ be given, in block form, by

$$J = \begin{pmatrix} 0 & \mathrm{Id} \\ -\mathrm{Id} & 0 \end{pmatrix}, \qquad \Gamma = \begin{pmatrix} 0 & 0 \\ 0 & G^T\gamma G \end{pmatrix}, \qquad \Sigma = \begin{pmatrix} 0 \\ G^T\sigma \end{pmatrix}. \tag{3.54}$$

The next result shows that if $(r, \eta, p, \pi)(t)$ is a process satisfying the equations in (2.12) and (3.14), then the process $(r, \eta, \psi, \zeta)(t)$ satisfies a system of equations with a canonical Hamiltonian structure.

PROPOSITION 3.6. *Let $(r, \eta, p, \pi)(t)$ be any process satisfying the equations in* (2.12) *and* (3.14). *Then the process $(r, \eta, \psi, \zeta)(t)$ satisfies the canonical Hamilton–Langevin equations*

$$\dot{x} = \frac{\partial H}{\partial y}, \qquad \dot{y} = -\frac{\partial H}{\partial x} - G^T\gamma G\frac{\partial H}{\partial y} + G^T\sigma\dot{W}, \tag{3.55}$$

where $x = (r, \eta) \in \mathbb{R}^6$, $y = (\psi, \zeta) \in \mathbb{R}^6$, and $H(x, y) = \frac{1}{2}y \cdot G^{-1}M^{-1}G^{-T}y + U(x)$. Equivalently, introducing $z = (x, y) \in \mathbb{R}^{12}$, we have

$$\dot{z} = (J - \Gamma)\frac{\partial H}{\partial z} + \Sigma\dot{W}. \tag{3.56}$$

Proof. The result for $x = (r, \eta)$ follows directly from $(2.12)_1$, (3.14), and Proposition 3.3. To establish the result for $y = (\psi, \zeta)$, we notice first that $\psi = p$ by the third pair of equations in (3.33). Using $(2.12)_3$ and Proposition 3.3, we get

$$\dot{\psi} = -\frac{\partial \Psi}{\partial r} + f, \tag{3.57}$$

where $f = f^{(v)} + f^{(c)} + f^{(s)}$. Since ζ is a function of (r, η, p, π), (r, η) satisfy equations with no diffusion terms, and ζ is linear in (p, π), we find that Itô's formula reduces to the ordinary chain rule, which can be written as

$$\dot{\zeta}_i = \frac{\partial \zeta_i}{\partial r_k}\dot{r}_k + \frac{\partial \zeta_i}{\partial \eta_k}\dot{\eta}_k + \frac{\partial \zeta_i}{\partial p_k}\dot{p}_k + \frac{\partial \zeta_i}{\partial \pi_k}\dot{\pi}_k. \tag{3.58}$$

Combining this with the third pair of equations in (3.33), we get, using matrix notation,

$$\dot{\zeta} = \dot{S}^T\big(r \times p + \pi\big) + S^T\big(\dot{r} \times p + r \times \dot{p} + \dot{\pi}\big). \tag{3.59}$$

Substituting for $\dot{r}$, $\dot{p}$, and $\dot{\pi}$ from (2.12) and using the relation $v = m^{-1}p + c \times \omega$ from the first pair of equations in (3.33) and the vector identity $(x\times y)\times z = (x\cdot z)y - (y\cdot z)x$, we obtain

$$\dot{\zeta} = \dot{S}^T\big(r \times p + \pi\big) + S^T\big(\pi \times \omega + (r \times p) \times \omega\big) + S^T\big(r \times f + \tau\big), \tag{3.60}$$

where $\tau = \tau^{(v)} + \tau^{(c)} + \tau^{(s)}$. Writing the above result in components and using the relation $\dot{\eta}_j = [S^{-1}\omega]_j$ from (3.14), we get

$$\begin{aligned}\dot{\zeta}_l = \frac{\partial S_{ml}}{\partial \eta_j}\Big[S^{-1}\omega\Big]_j\Big[r\times p+\pi\Big]_m \\ + \Big[S^T\Big(\pi\times\omega+(r\times p)\times\omega\Big)\Big]_l + \Big[S^T\Big(r\times f+\tau\Big)\Big]_l,\end{aligned} \tag{3.61}$$

and from Proposition 3.3 we obtain, after converting back to matrix form,

$$\dot{\zeta} = -\frac{\partial \Psi}{\partial \eta} + S^T\big(r\times f+\tau\big). \tag{3.62}$$

The desired result for $y = (\psi, \zeta)$ follows by combining (3.57) and (3.62) and using Propositions 3.4 and 3.5 to substitute for the component vector (f, τ), that is,

$$\begin{aligned}\begin{pmatrix}\dot{\psi}\\ \dot{\zeta}\end{pmatrix} &= -\begin{pmatrix}\frac{\partial\Psi}{\partial r}\\ \frac{\partial\Psi}{\partial\eta}\end{pmatrix} + G^T\begin{pmatrix}f\\ \tau\end{pmatrix}\\ &= -\begin{pmatrix}\frac{\partial\Psi}{\partial r}\\ \frac{\partial\Psi}{\partial\eta}\end{pmatrix} + G^T\left[-G^{-T}\begin{pmatrix}\frac{\partial U}{\partial r}\\ \frac{\partial U}{\partial\eta}\end{pmatrix} - \gamma G\begin{pmatrix}\frac{\partial\Psi}{\partial\psi}\\ \frac{\partial\Psi}{\partial\zeta}\end{pmatrix} + \sigma\dot{W}\right]\\ &= -\begin{pmatrix}\frac{\partial H}{\partial r}\\ \frac{\partial H}{\partial\eta}\end{pmatrix} - G^T\gamma G\begin{pmatrix}\frac{\partial H}{\partial\psi}\\ \frac{\partial H}{\partial\zeta}\end{pmatrix} + G^T\sigma\dot{W}. \qquad \square\end{aligned} \tag{3.63}$$

3.5. Invariance of canonical formulation. Here we show that the Hamilton–Langevin equations in Proposition 3.6 are invariant under an arbitrary change of configuration variables provided that the new momentum variable is taken as the associated canonical one.

Let $x = (r, \eta)$ and $y = (\psi, \zeta)$ be as in Proposition 3.6 and consider new variables $\widetilde{x}$ and $\widetilde{y}$ defined by

$$\widetilde{x} = \phi(x), \qquad \widetilde{y} = D\phi^{-T}(x)y, \tag{3.64}$$

where $\phi(x)$ is an arbitrary bijective map with Jacobian matrix $D\phi(x)$. For brevity, we denote the above transformations by $\widetilde{x} = \widetilde{x}(x)$ and $\widetilde{y} = \widetilde{y}(x, y)$ and the inverse transformations by $x = x(\widetilde{x})$ and $y = y(\widetilde{x}, \widetilde{y})$. Analogous to (3.23), let $\widetilde{G}(\widetilde{x}) \in \mathbb{R}^{6\times 6}$ be the velocity structure matrix for the configuration variable $\widetilde{x}$ defined such that

$$\nu = \widetilde{G}\dot{\widetilde{x}}, \tag{3.65}$$

where $\nu = (v, \omega)$ are the body-frame components of the body linear and angular velocities.

The variable $\widetilde{y}$ defined in (3.64) can be identified as the canonical momentum associated with $\widetilde{x}$. In particular, from (3.23), $(3.64)_1$, and (3.65) we find

$$\widetilde{G} = G\,D\phi^{-1}, \tag{3.66}$$

and from (3.23), (3.31), $(3.64)_2$, (3.65), and (3.66) we deduce that

$$\widetilde{y} = \widetilde{G}^T M\widetilde{G}\dot{\widetilde{x}} = \frac{\partial\widetilde{T}}{\partial\dot{\widetilde{x}}}, \tag{3.67}$$

where $\widetilde{T}$ is the kinetic energy of the body expressed as a function of $(\widetilde{x}, \dot{\widetilde{x}})$, that is,

$$\widetilde{T}(\widetilde{x}, \dot{\widetilde{x}}) = \Phi(v, \omega)\Big|_{(v,\omega)=\widetilde{G}\dot{\widetilde{x}}} = \frac{1}{2}\dot{\widetilde{x}} \cdot \widetilde{G}^T M \widetilde{G} \dot{\widetilde{x}}. \tag{3.68}$$

Finally, let $\widetilde{H}(\widetilde{x}, \widetilde{y})$, $\widetilde{U}(\widetilde{x})$, $\widetilde{\gamma}(\widetilde{x})$, and $\widetilde{\sigma}(\widetilde{x})$ be functions defined via the change of variables as

$$\begin{aligned} \widetilde{H}(\widetilde{x}, \widetilde{y}) = H(x, y)|_{x=x(\widetilde{x}), y=y(\widetilde{x}, \widetilde{y})}, \qquad \widetilde{U}(\widetilde{x}) = U(x)|_{x=x(\widetilde{x})}, \\ \widetilde{\gamma}(\widetilde{x}) = \gamma(x)|_{x=x(\widetilde{x})}, \qquad \widetilde{\sigma}(\widetilde{x}) = \sigma(x)|_{x=x(\widetilde{x})}. \end{aligned} \tag{3.69}$$

The following result generalizes a classic result from the theory of Hamiltonian systems. It shows that, just as in the deterministic case, the form of the canonical equations in the stochastic case is invariant under the class of transformations in (3.64). In particular, if $(x, y)(t)$ is a process satisfying the system in (3.55), then the process $(\widetilde{x}, \widetilde{y})(t)$ satisfies a system of precisely the same form. Similar results for particle systems can be found in [23].

PROPOSITION 3.7. *Let $(x, y)(t)$ be any process satisfying the Hamilton–Langevin equations* (3.55)*. Then, after an arbitrary change of configuration variables, the process $(\widetilde{x}, \widetilde{y})(t)$ satisfies Hamilton–Langevin equations of the same form, namely*

$$\dot{\widetilde{x}} = \frac{\partial \widetilde{H}}{\partial \widetilde{y}}, \qquad \dot{\widetilde{y}} = -\frac{\partial \widetilde{H}}{\partial \widetilde{x}} - \widetilde{G}^T \widetilde{\gamma} \widetilde{G} \frac{\partial \widetilde{H}}{\partial \widetilde{y}} + \widetilde{G}^T \widetilde{\sigma} \dot{W}, \tag{3.70}$$

where $\widetilde{H}(\widetilde{x}, \widetilde{y}) = \frac{1}{2}\widetilde{y} \cdot \widetilde{G}^{-1} M^{-1} \widetilde{G}^{-T} \widetilde{y} + \widetilde{U}(\widetilde{x})$ is the total system energy, and $\widetilde{G}$ and $\widetilde{y}$ are the velocity structure matrix and canonical momentum associated with $\widetilde{x}$.

Proof. Since x satisfies an equation with no diffusion terms and the function $\widetilde{y} = \widetilde{y}(x, y)$ is linear in y, we find that Itô's formula applied to (3.64) reduces to the ordinary chain rule. Thus in components, employing the usual summation convention, we have

$$\dot{\widetilde{x}}_i = \frac{\partial \widetilde{x}_i}{\partial x_j} \dot{x}_j, \qquad \dot{\widetilde{y}}_i = \frac{\partial \widetilde{y}_i}{\partial x_j} \dot{x}_j + \frac{\partial \widetilde{y}_i}{\partial y_j} \dot{y}_j, \tag{3.71}$$

where indices take values from one through six. From $(3.69)_1$ we get $H(x, y) = \widetilde{H}(\widetilde{x}, \widetilde{y})|_{\widetilde{x}=\widetilde{x}(x), \widetilde{y}=\widetilde{y}(x,y)}$, which implies

$$\frac{\partial H}{\partial x_j} = \frac{\partial \widetilde{H}}{\partial \widetilde{x}_k} \frac{\partial \widetilde{x}_k}{\partial x_j} + \frac{\partial \widetilde{H}}{\partial \widetilde{y}_k} \frac{\partial \widetilde{y}_k}{\partial x_j}, \qquad \frac{\partial H}{\partial y_j} = \frac{\partial \widetilde{H}}{\partial \widetilde{y}_k} \frac{\partial \widetilde{y}_k}{\partial y_j}. \tag{3.72}$$

Substituting $(3.55)_1$ and $(3.72)_2$ into $(3.71)_1$ and using the relations $\partial \widetilde{x}/\partial x = D\phi$ and $\partial \widetilde{y}/\partial y = D\phi^{-T}$, we obtain

$$\dot{\widetilde{x}}_i = [D\phi]_{ij} [D\phi^{-T}]_{kj} \frac{\partial \widetilde{H}}{\partial \widetilde{y}_k} = \frac{\partial \widetilde{H}}{\partial \widetilde{y}_i}, \tag{3.73}$$

which establishes the result for $\widetilde{x}$. Substituting $(3.55)_2$ and (3.72) into $(3.71)_2$ and using $\partial \widetilde{x}/\partial x = D\phi$ and $\partial \widetilde{y}/\partial y = D\phi^{-T}$, together with (3.66) and (3.69), we get

$$\dot{\widetilde{y}}_i = \frac{\partial \widetilde{y}_i}{\partial x_j} \dot{x}_j - \frac{\partial \widetilde{y}_i}{\partial y_j} \frac{\partial \widetilde{H}}{\partial \widetilde{y}_k} \frac{\partial \widetilde{y}_k}{\partial x_j} - \frac{\partial \widetilde{H}}{\partial \widetilde{x}_i} - \left[\widetilde{G}^T \widetilde{\gamma} \widetilde{G} \frac{\partial \widetilde{H}}{\partial \widetilde{y}} \right]_i + [\widetilde{G}^T \widetilde{\sigma} \dot{W}]_i. \tag{3.74}$$

Since $\partial \widetilde{H}/\partial \widetilde{y} = \dot{\widetilde{x}}$ and $\widetilde{x} = \widetilde{x}(x)$, we can rewrite (3.74) as

$$\dot{\widetilde{y}}_i = \left(\frac{\partial \widetilde{y}_i}{\partial x_m} - \frac{\partial \widetilde{y}_i}{\partial y_j}\frac{\partial \widetilde{x}_k}{\partial x_m}\frac{\partial \widetilde{y}_k}{\partial x_j}\right)\dot{x}_m - \frac{\partial \widetilde{H}}{\partial \widetilde{x}_i} - \left[\widetilde{G}^T\widetilde{\gamma}\widetilde{G}\frac{\partial \widetilde{H}}{\partial \widetilde{y}}\right]_i + [\widetilde{G}^T\widetilde{\sigma}\dot{W}]_i. \tag{3.75}$$

The coefficient of $\dot{x}_m$ in the above equation vanishes. To see this, we use the relation $\widetilde{y} = D\phi^{-T}(x)y$ to write

$$\frac{\partial \widetilde{y}_i}{\partial y_j}\frac{\partial \widetilde{x}_k}{\partial x_m}\frac{\partial \widetilde{y}_k}{\partial x_j} = [D\phi^{-T}]_{ij}\frac{\partial \widetilde{x}_k}{\partial x_m}\left(\frac{\partial}{\partial x_j}[D\phi^{-T}]_{kp}\right)y_p. \tag{3.76}$$

From the relation $\widetilde{x} = \phi(x)$ we have $[D\phi^{-T}]_{ln} = \partial x_n/\partial \widetilde{x}_l$, and using this in (3.76) together with the chain rule and symmetry of second partial derivatives we find

$$\begin{aligned}\frac{\partial \widetilde{y}_i}{\partial y_j}\frac{\partial \widetilde{x}_k}{\partial x_m}\frac{\partial \widetilde{y}_k}{\partial x_j} &= \frac{\partial x_j}{\partial \widetilde{x}_i}\frac{\partial \widetilde{x}_k}{\partial x_m}\left(\frac{\partial}{\partial x_j}\frac{\partial x_p}{\partial \widetilde{x}_k}\right)y_p \\ &= \frac{\partial \widetilde{x}_k}{\partial x_m}\left(\frac{\partial}{\partial \widetilde{x}_i}\frac{\partial x_p}{\partial \widetilde{x}_k}\right)y_p = \left(\frac{\partial}{\partial x_m}\frac{\partial x_p}{\partial \widetilde{x}_i}\right)y_p = \frac{\partial \widetilde{y}_i}{\partial x_m}.\end{aligned} \tag{3.77}$$

Substituting (3.77) into (3.75) we obtain

$$\dot{\widetilde{y}}_i = -\frac{\partial \widetilde{H}}{\partial \widetilde{x}_i} - \left[\widetilde{G}^T\widetilde{\gamma}\widetilde{G}\frac{\partial \widetilde{H}}{\partial \widetilde{y}}\right]_i + [\widetilde{G}^T\widetilde{\sigma}\dot{W}]_i, \tag{3.78}$$

which establishes the result for $\widetilde{y}$. □

3.6. Noncanonical Hamilton–Langevin formulation. Consider configuration variables (r, η) with physical momenta variables (p, π), and consider the Hamiltonian function defined by

$$H^{\mathrm{nc}}(r, \eta, p, \pi) = \Upsilon(r, \eta, p, \pi) + U(r, \eta), \tag{3.79}$$

where $\Upsilon(r, \eta, p, \pi)$ and $U(r, \eta)$ are the kinetic and potential energy functions. Let $J^{\mathrm{nc}} = J^{\mathrm{nc}}(r, \eta, p, \pi) \in \mathbb{R}^{12\times 12}$, $E = E(p, \pi) \in \mathbb{R}^{6\times 6}$, $\Gamma^{\mathrm{nc}} = \Gamma^{\mathrm{nc}}(r, \eta) \in \mathbb{R}^{12\times 12}$, and $\Sigma^{\mathrm{nc}} = \Sigma^{\mathrm{nc}}(r, \eta) \in \mathbb{R}^{12\times 6}$ be given, in block form, by

$$\begin{aligned} J^{\mathrm{nc}} &= \begin{pmatrix} 0 & G^{-1} \\ -G^{-T} & E \end{pmatrix}, \qquad E = \begin{pmatrix} 0 & [p\times] \\ [p\times] & [\pi\times] \end{pmatrix}, \\ \Gamma^{\mathrm{nc}} &= \begin{pmatrix} 0 & 0 \\ 0 & \gamma \end{pmatrix}, \qquad \Sigma^{\mathrm{nc}} = \begin{pmatrix} 0 \\ \sigma \end{pmatrix}. \end{aligned} \tag{3.80}$$

The next result, which follows by inspection from Propositions 3.3, 3.4, and 3.5, shows that the equations in (2.12) and (3.14) for the process $(r, \eta, p, \pi)(t)$ possess a natural noncanonical Hamiltonian structure.

PROPOSITION 3.8. *Equations* (2.12) *and* (3.14) *for the process* $(r, \eta, p, \pi)(t)$ *can be written in the noncanonical Hamilton–Langevin form*

$$\dot{x} = G^{-1}\frac{\partial H^{\mathrm{nc}}}{\partial y^{\mathrm{nc}}}, \qquad \dot{y}^{\mathrm{nc}} = -G^{-T}\frac{\partial H^{\mathrm{nc}}}{\partial x} + E\frac{\partial H^{\mathrm{nc}}}{\partial y^{\mathrm{nc}}} - \gamma\frac{\partial H^{\mathrm{nc}}}{\partial y^{\mathrm{nc}}} + \sigma\dot{W}, \tag{3.81}$$

where $x = (r, \eta) \in \mathbb{R}^6$, $y^{\mathrm{nc}} = (p, \pi) \in \mathbb{R}^6$, *and* $H^{\mathrm{nc}}(x, y^{\mathrm{nc}}) = \frac{1}{2}y^{\mathrm{nc}} \cdot M^{-1}y^{\mathrm{nc}} + U(x)$. *Equivalently, introducing* $z^{\mathrm{nc}} = (x, y^{\mathrm{nc}}) \in \mathbb{R}^{12}$, *we have*

$$\dot{z}^{\mathrm{nc}} = (J^{\mathrm{nc}} - \Gamma^{\mathrm{nc}})\frac{\partial H^{\mathrm{nc}}}{\partial z^{\mathrm{nc}}} + \Sigma^{\mathrm{nc}}\dot{W}. \tag{3.82}$$

This formulation will be useful later in interpreting a certain factorization of the standard canonical measure associated with the canonical formulation in Proposition 3.6.

3.7. Invariance of noncanonical formulation. Here we show that, just as in the canonical case, the noncanonical Hamilton–Langevin equations in Proposition 3.8 are invariant under an arbitrary change of configuration variables.

Let $x = (r, \eta)$ and $y^{\mathrm{nc}} = (p, \pi)$ be as in Proposition 3.8 and consider a new configuration variable $\widetilde{x}$ defined as in (3.64), with associated velocity structure matrix $\widetilde{G}(\widetilde{x}) \in \mathbb{R}^{6\times 6}$ defined as in (3.65). Moreover, let $\widetilde{H}^{\mathrm{nc}}(\widetilde{x}, y^{\mathrm{nc}})$, $\widetilde{U}(\widetilde{x})$, $\widetilde{\gamma}(\widetilde{x})$, and $\widetilde{\sigma}(\widetilde{x})$ be functions defined via the change of variables as

$$\begin{aligned} \widetilde{H}^{\mathrm{nc}}(\widetilde{x}, y^{\mathrm{nc}}) = H^{\mathrm{nc}}(x, y^{\mathrm{nc}})|_{x=x(\widetilde{x})}, \qquad \widetilde{U}(\widetilde{x}) = U(x)|_{x=x(\widetilde{x})}, \\ \widetilde{\gamma}(\widetilde{x}) = \gamma(x)|_{x=x(\widetilde{x})}, \qquad \widetilde{\sigma}(\widetilde{x}) = \sigma(x)|_{x=x(\widetilde{x})}. \end{aligned} \tag{3.83}$$

Notice that the noncanonical momentum y^{nc} and coefficient matrix E in (3.81) are not affected by the change of configuration variables from x to $\widetilde{x}$.

The following result extends Proposition 3.7 to the noncanonical case. In particular, if $(x, y^{\mathrm{nc}})(t)$ is a process satisfying the system in (3.81), then the process $(\widetilde{x}, y^{\mathrm{nc}})(t)$ satisfies a system of precisely the same form. The proof is similar to that of Proposition 3.7 and is omitted for brevity.

PROPOSITION 3.9. *Let $(x, y^{\mathrm{nc}})(t)$ be any process satisfying the noncanonical Hamilton–Langevin equations* (3.81)*. Then, after an arbitrary change of configuration variables, the process $(\widetilde{x}, y^{\mathrm{nc}})(t)$ satisfies noncanonical Hamilton–Langevin equations of the same form, namely*

$$\dot{\widetilde{x}} = \widetilde{G}^{-1}\frac{\partial \widetilde{H}^{\mathrm{nc}}}{\partial y^{\mathrm{nc}}}, \qquad \dot{y}^{\mathrm{nc}} = -\widetilde{G}^{-T}\frac{\partial \widetilde{H}^{\mathrm{nc}}}{\partial \widetilde{x}} + E\frac{\partial \widetilde{H}^{\mathrm{nc}}}{\partial y^{\mathrm{nc}}} - \widetilde{\gamma}\frac{\partial \widetilde{H}^{\mathrm{nc}}}{\partial y^{\mathrm{nc}}} + \widetilde{\sigma}\dot{W}, \tag{3.84}$$

where $\widetilde{H}^{\mathrm{nc}}(\widetilde{x}, y^{\mathrm{nc}}) = \frac{1}{2} y^{\mathrm{nc}} \cdot M^{-1} y^{\mathrm{nc}} + \widetilde{U}(\widetilde{x})$ is the total system energy and $\widetilde{G}$ is the velocity structure matrix associated with $\widetilde{x}$.

4. Measures for Hamiltonian formulations. Here we study various measures associated with the Hamilton–Langevin system in (3.55). We introduce the canonical measure associated with this system, outline conditions under which the measure is stationary, and discuss various issues that arise in a rigid body model. We then show that the canonical measure can always be factorized into independent measures on configuration and velocity space, and we interpret this factorization in terms of the noncanonical system in (3.81). Moreover, we show that the canonical, configuration, and velocity measures are each invariant under an arbitrary change of configuration variables.

4.1. Fokker–Planck description. Consider the Hamilton–Langevin system in (3.55), where $x = (r, \eta)$, $y = (\psi, \zeta)$, and $z = (x, y)$. We denote the spaces for x, y, and z by $\mathcal{X}$, $\mathcal{Y}$, and $\mathcal{Z}$ and note that $\mathcal{X} = \mathbb{R}^3 \times \mathcal{A} \subset \mathbb{R}^6$, $\mathcal{Y} = \mathbb{R}^3 \times \mathbb{R}^3 = \mathbb{R}^6$, and $\mathcal{Z} = \mathcal{X} \times \mathcal{Y} \subset \mathbb{R}^{12}$. For any given initial condition z_0, or distribution thereof, and any time $t > 0$, we assume that the random variable $z(t)$ defined by (3.55) is distributed according to a normalized (probability) measure μ_t so that for any open set $\mathcal{O} \subset \mathcal{Z}$ we have $\Pr\{z(t) \in \mathcal{O}\} = \int_{\mathcal{O}} \mu_t(dz)$. Moreover, we assume that μ_t is absolutely continuous with respect to the Lebesgue measure in the sense that $\mu_t(dz) = \varphi(z, t)\, dz$ for some density function $\varphi(z, t)$.

According to the theory of Itô stochastic differential equations, the density φ satisfies the Fokker–Planck equation [18, 31, 45, 49], which (using the summation convention) takes the form

$$\frac{\partial \varphi}{\partial t} = -\frac{\partial}{\partial z_i}\left[A_i \varphi\right] + \frac{1}{2}\frac{\partial^2}{\partial z_i \partial z_j}\left[B_{ij}\varphi\right], \qquad z \in \mathcal{Z}, \qquad t > 0. \tag{4.1}$$

Here indices take values from 1 through 12, and $A = A(z) \in \mathbb{R}^{12}$ and $B = B(z) \in \mathbb{R}^{12\times 12}$ are coefficients defined by

$$A = (J - \Gamma)\frac{\partial H}{\partial z}, \qquad B = \Sigma\Sigma^T. \tag{4.2}$$

The spatial terms on the right-hand side of (4.1) can be written as the negative divergence of a probability current or flux field $F = F(z) \in \mathbb{R}^{12}$ defined as

$$F_i = A_i\varphi - \frac{1}{2}\frac{\partial}{\partial z_j}\left[B_{ij}\varphi\right]. \tag{4.3}$$

Appropriate boundary conditions for (4.1) can be specified as follows. For notational convenience, consider writing $\mathcal{Z}$ as the Cartesian product of bounded or unbounded open intervals (a_i, b_i) $(i = 1, \ldots, 12)$, and let $N|_{z_i=a_i} \in \mathbb{R}^{12}$ and $N|_{z_i=b_i} \in \mathbb{R}^{12}$ denote the standard unit vectors which are normal to the coordinate hyperplanes $z_i = a_i$ and $z_i = b_i$, including points at infinity, oriented outwardly from $\mathcal{Z}$. Moreover, let $\mathcal{I}^{\text{mom}}$, $\mathcal{I}^{\text{con}}_{\text{cyclic}}$, and $\mathcal{I}^{\text{con}}_{\text{acyclic}}$ denote the sets of indices i for which z_i is a momentum coordinate, cyclic configuration coordinate, and acyclic configuration coordinate, where all translational coordinates are grouped in the acyclic set. Then appropriate boundary conditions are [18, 45]

$$F \cdot N|_{z_i=a_i} = 0, \qquad F \cdot N|_{z_i=b_i} = 0, \qquad i \in \mathcal{I}^{\text{mom}} \cup \mathcal{I}^{\text{con}}_{\text{acyclic}}, \tag{4.4}$$

$$F \cdot N|_{z_i=a_i} = -F \cdot N|_{z_i=b_i}, \qquad i \in \mathcal{I}^{\text{con}}_{\text{cyclic}}. \tag{4.5}$$

The conditions in (4.4) state that the normal current at the boundary of $\mathcal{Z}$ is zero for each of the momentum and acyclic configuration coordinates; that is, there are no probability leaks. The conditions in (4.5) state that the normal current at the boundary of $\mathcal{Z}$ is periodic for each of the cyclic configuration coordinates; the minus sign arises because $N|_{z_i=a_i} = -N|_{z_i=b_i}$. Each condition should be understood to hold almost everywhere on the indicated hyperplane, or a portion thereof, defined by all points in $\mathcal{Z}$ with the specified value of z_i. In (4.5), points on the opposing, parallel hyperplanes $z_i = b_i$ and $z_i = a_i$ are identified with each other in the obvious way.

Various assumptions are required in order for (4.4) and (4.5) to be meaningful. For (4.4), we assume that the approach to a boundary value of zero, obtained by taking limits from the interior of $\mathcal{Z}$, occurs sufficiently fast so that the surface integrals of $F \cdot N$ over the indicated hyperplanes converge. Similarly, for (4.5), we assume that the surface integrals of $F \cdot N$ over each pair of opposing hyperplanes also converge. In this case, the conditions imply that the total probability is conserved for all $t > 0$. This can be verified by integrating (4.1) over a sequence of bounded interior domains of increasing size, applying the divergence theorem to each, and taking limits.

4.2. Canonical measure. We consider a time-independent measure μ on $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ of the form

$$\mu(dz) = \rho(z)\, dz, \qquad \rho(z) = \frac{1}{C}e^{-\beta H(z)}, \tag{4.6}$$

where β and C are fixed, positive constants. We will consider only the case when μ is normalizable, or equivalently $\int_{\mathcal{Z}} e^{-\beta H}\, dz$ is finite, and choose C to obtain a probability measure. When the stochastic forcing in (3.55) is meant to model a heat bath at absolute temperature Θ, we take $\beta = 1/(\kappa\Theta)$, where κ is the Boltzmann constant. In this case, we call μ and ρ the canonical measure and density associated with (3.55).

The connection between the canonical measure and Hamilton–Langevin equations is a well-studied subject; see, for example, the treatise [49] and references therein. Here we outline a standard result, commonly referred to as the fluctuation-dissipation theorem [18, 29, 31, 45], which establishes sufficient conditions for the canonical measure to be stationary under the dynamics described by (3.55) or, equivalently, (4.1). We remark that, in contrast to the classic case of particle systems on unbounded domains, for which boundary conditions need not be considered, the case of rigid bodies as developed here requires their consideration. The proof of the result is straightforward and is omitted for brevity.

PROPOSITION 4.1. *Consider the canonical Hamilton–Langevin equations* (3.55) *and assume the following:*

A1. *the integral* $\int_{\mathcal{Z}} e^{-\beta H}\,dz$ *is finite, and the vector field* $J\frac{\partial e^{-\beta H}}{\partial z}$ *satisfies* (4.4) *and* (4.5) *on the boundary of* $\mathcal{Z}$*;*

A2. *the resistance matrix* γ *and noise matrix* σ *satisfy* $2\gamma = \beta\sigma\sigma^T$ *at all points in* $\mathcal{Z}$*.*

Then the canonical density ρ *is a stationary or steady-state solution of the Fokker–Planck equation* (4.1) *subject to the boundary conditions* (4.4) *and* (4.5)*.*

Motivated by Proposition 4.1, we say that a system is in thermal equilibrium at temperature Θ if its states z are distributed according to the canonical measure μ. The proposition implies that, under suitable constitutive assumptions on H, γ, and σ, a system which is in thermal equilibrium at $t = 0$ will remain so for all $t > 0$. As a consequence, the expected or average value of any state function $f(z)$ is independent of time and is given by

$$\mathbb{E}_\mu[f] = \int_{\mathcal{Z}} f(z)\,\mu(dz). \tag{4.7}$$

Remarks 4.1.

1. Assumption A1 requires that the Hamiltonian satisfy appropriate periodicity and asymptotic growth conditions. It must be periodic in the cyclic configuration coordinates (if any) and grow sufficiently rapidly in the momentum and acyclic configuration coordinates. The periodicity condition is straightforward; it is sufficient for the potential energy in local coordinates to be the representation of a function on the intrinsic configuration space $\mathbb{R}^3 \times SO_3$. The growth condition is more complicated; it depends on properties of both the kinetic and the potential energies and on the coordinate chart for SO_3 through the velocity structure matrix.
2. Finiteness of the integral $\iint_{\mathcal{X}\times\mathcal{Y}} e^{-\beta H(x,y)}\,dx\,dy$ can be achieved without a growth condition on the rotational component of the potential $U(x)$. Indeed, performing the Gaussian integral over $\mathcal{Y}$ and using Proposition 3.1(iii) and the relation $|G(x)| = |S(\eta)|$, we find

$$\begin{aligned}\iint_{\mathcal{X}\times\mathcal{Y}} e^{-\beta H(x,y)}\,dx\,dy &= (2\pi/\beta)^3\sqrt{|M|}\int_{\mathcal{X}} e^{-\beta U(x)}|G(x)|\,dx \\ &= (2\pi/\beta)^3\sqrt{|M|}\iint_{\mathbb{R}^3\times\mathcal{A}} e^{-\beta U(r,\eta)}|S(\eta)|\,dr\,d\eta \\ &= (\sqrt{2}\pi/\beta)^3\sqrt{|M|}\iint_{\mathbb{R}^3\times SO_3} e^{-\beta U(r,\eta(Q))}\,dr\,dQ.\end{aligned} \tag{4.8}$$

From this we deduce, by compactness of SO_3, that the integral will be finite if $U(r,\eta)$ is bounded from below for all (r,η) and satisfies a growth condition in r. In particular, no growth is required in η, even if the domain $\mathcal{A}$ is unbounded.

3. There are some advantages to using a Cayley chart for SO_3 in the modeling of bodies with strongly restrained degrees of freedom. Indeed, because all rotational coordinates are acyclic, the potential need not satisfy any periodicity conditions. Thus an arbitrary, fully coupled potential energy could be modeled using a simple functional form, for example, a positive-definite, quadratic function of all the coordinates, which presumably would be sufficient to satisfy assumption A1. Such a form will be employed in the multibody model of a polymer chain introduced later, where the translational and rotational coordinates will describe the relative displacements and rotations between bodies.
4. Assumption A2 requires that the matrices γ and σ satisfy a constitutive relation. In a standard Stokesian model of viscous loads, γ would be a symmetric, positive-definite matrix uniquely determined by the geometry of the body, and σ would be a necessarily invertible matrix determined from the relation $\beta\sigma\sigma^T = 2\gamma$. Although this relation does not uniquely determine σ, any solution is sufficient to guarantee the stationarity of the measure μ. The symmetry, definiteness, and invertibility of γ and σ extend to the coefficient matrices $G^T\gamma G$ and $G^T\sigma$ appearing in (3.55), but not uniformly so. Indeed, while $|G|$ is nonzero at all points in $\mathcal{Z}$, nonuniformity arises because $|G|$ may vanish at boundary points.
5. A detailed analysis of ergodicity for (3.55) is beyond the scope of this article. Nevertheless, in the case when γ is symmetric and positive-definite, and σ is invertible, we expect the stationary measure μ to be unique and consequently [44] solutions of (3.55) to be ergodic with respect to μ in the sense that

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T f(z(t))\,dt = \int_{\mathcal{Z}} f(z)\,\mu(dz), \tag{4.9}$$

where the equality is understood to hold for almost every sample path $z(t)$. We remark that the stronger notion of geometric ergodicity has recently been established for related systems and their numerical approximation under various different assumptions [36, 37, 50].

4.3. Invariance of canonical measure. Consider a change of variables from $(x,y) \in \mathcal{X}\times\mathcal{Y}$ to $(\widetilde{x},\widetilde{y}) \in \widetilde{\mathcal{X}}\times\widetilde{\mathcal{Y}}$ defined as in (3.64), where $\phi : \mathcal{X} \to \widetilde{\mathcal{X}}$ is an arbitrary bijection. For a fixed temperature Θ, let μ and $\widetilde{\mu}$ be the canonical measures associated with (3.55) and (3.70), so that

$$\mu(dx,dy) = \frac{1}{C}e^{-\beta H(x,y)}\,dx\,dy, \qquad \widetilde{\mu}(d\widetilde{x},d\widetilde{y}) = \frac{1}{\widetilde{C}}e^{-\beta \widetilde{H}(\widetilde{x},\widetilde{y})}\,d\widetilde{x}\,d\widetilde{y}. \tag{4.10}$$

The next result, which is well known and included only for completeness, can be understood as a consequence of Proposition 3.7. It shows that the measures μ and $\widetilde{\mu}$ are equivalent in the sense that they both yield the same expected value for any given state function. That is, the canonical measure is invariant under the change of variables (3.64). The proof is straightforward and relies on the fact that the Jacobian determinant of this change of variables is identically equal to one.

PROPOSITION 4.2. *Let $\mathbb{E}_\mu$ and $\mathbb{E}_{\widetilde{\mu}}$ denote expectations with respect to μ and $\widetilde{\mu}$. Then for any state function $f(x,y)$ we have*

$$\mathbb{E}_{\widetilde{\mu}}[\widetilde{f}] = \mathbb{E}_\mu[f], \tag{4.11}$$

where $\widetilde{f}(\widetilde{x},\widetilde{y}) = f(x,y)|_{x=x(\widetilde{x}),y=y(\widetilde{x},\widetilde{y})}$.

The above result shows that the canonical measure, and hence the expected value of any state function, is an intrinsic property of the system described by (3.55). That is, these quantities are independent of the choice of configuration variables for the system, which in turn determines the conjugate momenta via (3.64).

4.4. Factorized measures. In general, due to the form of the Hamiltonian in (3.55), the canonical measure μ over the variables $(x,y) \in \mathcal{X} \times \mathcal{Y}$ cannot be readily factored into independent measures over the configuration variables $x = (r,\eta) \in \mathcal{X}$ and conjugate momentum variables $y = (\psi,\zeta) \in \mathcal{Y}$. However, here we show that μ can always be factored into independent measures over $x = (r,\eta) \in \mathcal{X}$ and $\nu = (v,\omega) \in \mathcal{V} = \mathbb{R}^6$, where (v,ω) are the body velocity components.

For a given potential energy $U(x)$ and kinetic energy $\Phi(\nu) = \frac{1}{2}\nu \cdot M\nu$ consider measures on $\mathcal{X}$ and $\mathcal{V}$ defined by

$$\mu^{\mathrm{con}}(dx) = \frac{1}{C'} e^{-\beta U(x)} |G(x)|\, dx, \qquad \mu^{\mathrm{vel}}(d\nu) = \frac{1}{C''} e^{-\beta \Phi(\nu)}\, d\nu, \tag{4.12}$$

where $\beta = 1/(\kappa\Theta)$, C' and C'' are positive constants, and $|G(x)|$ denotes the determinant of the velocity structure matrix $G(x)$ given in (3.23). Just as before, we assume that μ^{con} and μ^{vel} are normalizable and choose C' and C'' to obtain probability measures on $\mathcal{X}$ and $\mathcal{V}$. We call μ^{con} the canonical configuration measure and μ^{vel} the velocity measure associated with (3.55). Moreover, in view of (3.23) and (3.31), consider the change of variables from $(x,y) \in \mathcal{X} \times \mathcal{Y}$ to $(x,\nu) \in \mathcal{X} \times \mathcal{V}$ defined by

$$(x,y) = \chi(x,\nu) = (x, G^T(x) M\nu). \tag{4.13}$$

The next result follows from the fact that (4.13) separates the Hamiltonian in the sense that $H \circ \chi(x,\nu) = \Phi(\nu) + U(x)$ and has a simple Jacobian determinant given by $|\frac{\partial(x,y)}{\partial(x,\nu)}| = |G^T M|$.

PROPOSITION 4.3. *Under the change of variables* (4.13) *the canonical measure $\mu(dx,dy)$ is equivalent to the product measure $\mu^{\mathrm{con}}(dx)\mu^{\mathrm{vel}}(d\nu)$. That is, for any state function $f(x,y)$ we have*

$$\iint_{\mathcal{X}\times\mathcal{Y}} f(x,y)\, \mu(dx,dy) = \iint_{\mathcal{X}\times\mathcal{V}} f \circ \chi(x,\nu)\ \mu^{\mathrm{con}}(dx)\mu^{\mathrm{vel}}(d\nu). \tag{4.14}$$

The above result shows that, for a system in thermal equilibrium at temperature Θ, its configuration and velocity states (x,ν) are distributed according to the independent measures μ^{con} and μ^{vel}. That is, x and ν are statistically independent. As a consequence, the expected or average value of any functions $g(x)$ and $h(\nu)$ are given by

$$\mathbb{E}_{\mu^{\mathrm{con}}}[g] = \int_{\mathcal{X}} g(x)\, \mu^{\mathrm{con}}(dx), \qquad \mathbb{E}_{\mu^{\mathrm{vel}}}[h] = \int_{\mathcal{V}} h(\nu)\, \mu^{\mathrm{vel}}(d\nu). \tag{4.15}$$

As we will see later, the formulas in (4.15) will be useful in characterizing parameters in the energy functions $U(x)$ and $\Phi(\nu)$ under appropriate assumptions.

It is interesting to note that, under the conditions of Proposition 4.1, the product measure $\mu^{\mathrm{con}}\mu^{\mathrm{vel}}$ on $\mathcal{X}\times\mathcal{V}$ can be viewed as a stationary measure for the noncanonical formulation in (3.81), where the noncanonical momentum variable y^{nc} should be replaced by the velocity variable ν through the simple relation $y^{\mathrm{nc}} = M\nu$. Indeed, the stationarity of $\mu^{\mathrm{con}}\mu^{\mathrm{vel}}$ on $\mathcal{X}\times\mathcal{V}$ follows from the stationarity of μ on $\mathcal{X}\times\mathcal{Y}$ and the fact that (3.81) and (3.55) are connected, up to the relation $y^{\mathrm{nc}} = M\nu$, through the same change of variables which connects $\mu^{\mathrm{con}}\mu^{\mathrm{vel}}$ and μ.

4.5. Invariance of factorized measures. Consider a change of variables from $(x,y)\in\mathcal{X}\times\mathcal{Y}$ to $(\widetilde{x},\widetilde{y})\in\widetilde{\mathcal{X}}\times\widetilde{\mathcal{Y}}$ defined as in (3.64), where $\phi:\mathcal{X}\to\widetilde{\mathcal{X}}$ is an arbitrary bijection. For a fixed temperature Θ, let μ^{con} and $\widetilde{\mu}^{\mathrm{con}}$ be the canonical configuration measures associated with (3.55) and (3.70), so that

$$\mu^{\mathrm{con}}(dx) = \frac{1}{C'}e^{-\beta U(x)}\,|G(x)|\,dx, \qquad \widetilde{\mu}^{\mathrm{con}}(d\widetilde{x}) = \frac{1}{\widetilde{C}'}e^{-\beta\widetilde{U}(\widetilde{x})}\,|\widetilde{G}(\widetilde{x})|\,d\widetilde{x}. \tag{4.16}$$

Moreover, let μ^{vel} be the associated velocity measure given by

$$\mu^{\mathrm{vel}}(d\nu) = \frac{1}{C''}e^{-\beta\Phi(\nu)}\,d\nu. \tag{4.17}$$

By virtue of its definition, notice that μ^{vel} is independent of the choice of canonical variables.

The next result, which can be understood as a consequence of Proposition 3.9, shows that the measures μ^{con} and $\widetilde{\mu}^{\mathrm{con}}$ are equivalent in the sense that they both yield the same expected value for any given function. That is, the canonical configuration measure is invariant under an arbitrary change of configuration variables. The proof is straightforward and follows directly from Proposition 4.2 by choosing the arbitrary function $f(x,y)$ to be independent of y and then integrating over y.

PROPOSITION 4.4. *Let $\mathbb{E}_{\mu^{\mathrm{con}}}$ and $\mathbb{E}_{\widetilde{\mu}^{\mathrm{con}}}$ denote expectations with respect to μ^{con} and $\widetilde{\mu}^{\mathrm{con}}$. Then for any function $g(x)$ we have*

$$\mathbb{E}_{\widetilde{\mu}^{\mathrm{con}}}[\widetilde{g}] = \mathbb{E}_{\mu^{\mathrm{con}}}[g], \tag{4.18}$$

where $\widetilde{g}(\widetilde{x}) = g(x)|_{x=x(\widetilde{x})}$.

The above result shows that the canonical configuration measure μ^{con}, and hence the expected value of any configuration function $g(x)$, is an intrinsic property of the system described by (3.55). That is, these quantities are independent of the choice of configuration variables x for the system. The validity of this result depends crucially on the Jacobian factor $|G(x)|$ appearing in μ^{con}. Indeed, if this factor were omitted, the measure would in general not be invariant, and the expected value of a function would in general depend on the choice of variables.

5. Extension to systems. Here we extend our results from a single body to an arbitrary system of interacting rigid bodies. We describe how all results pertaining to the Hamiltonian form of the equations of motion and the associated canonical measures on phase, configuration, and velocity space carry over to systems. Throughout this section the summation convention remains in effect on subscripts i, j, and so on, but it is not employed on superscripts a, b, and so on.

5.1. General kinematics, balance laws. Consider a system of n independent rigid bodies with reference points $\boldsymbol{r}^a$ and body frames $\{\boldsymbol{d}_i^a\}$ $(a=1,\dots,n)$. Just as

in the case of a single body, the kinematics of each body a are encapsulated in the relations

$$\dot{\boldsymbol{r}}^a = \boldsymbol{v}^a, \qquad \dot{\boldsymbol{d}}_i^a = \boldsymbol{\omega}^a \times \boldsymbol{d}_i^a, \tag{5.1}$$

where $\boldsymbol{v}^a$ is the velocity of the reference point and $\boldsymbol{\omega}^a$ is the angular velocity of the body frame. Moreover, the momentum variables for each body a are defined by

$$\boldsymbol{p}^a = m^a(\boldsymbol{v}^a + \boldsymbol{\omega}^a \times \boldsymbol{c}^a), \qquad \boldsymbol{\pi}^a = \boldsymbol{I}^a\boldsymbol{\omega}^a + \boldsymbol{c}^a \times \boldsymbol{p}^a, \tag{5.2}$$

where $\boldsymbol{p}^a$ is the linear momentum, $\boldsymbol{\pi}^a$ is the angular momentum about the reference point, m^a is the total mass, $\boldsymbol{I}^a$ is the rotational inertia tensor with respect to the center of mass, and $\boldsymbol{c}^a$ is a vector from the reference point to the center of mass. Notice that $\boldsymbol{v}^a + \boldsymbol{\omega}^a \times \boldsymbol{c}^a$ on the right-hand side of $(5.2)_1$ is the velocity of the center of mass. Furthermore, the balance laws of linear and angular momenta for each body a take the form

$$\dot{\boldsymbol{p}}^a = \boldsymbol{f}^a, \qquad \dot{\boldsymbol{\pi}}^a = (\boldsymbol{\omega}^a \times \boldsymbol{c}^a) \times \boldsymbol{p}^a + \boldsymbol{\tau}^a, \tag{5.3}$$

where $\boldsymbol{f}^a$ is the resultant force and $\boldsymbol{\tau}^a$ is the resultant torque about the reference point of the body.

5.2. Resultant loads. We suppose that the resultant loads $(\boldsymbol{f}^a, \boldsymbol{\tau}^a)$ for each body a can be decomposed as

$$\boldsymbol{f}^a = \boldsymbol{f}^{a(v)} + \boldsymbol{f}^{a(c)} + \boldsymbol{f}^{a(s)}, \qquad \boldsymbol{\tau}^a = \boldsymbol{\tau}^{a(v)} + \boldsymbol{\tau}^{a(c)} + \boldsymbol{\tau}^{a(s)}, \tag{5.4}$$

where $(\boldsymbol{f}^{a(v)}, \boldsymbol{\tau}^{a(v)})$, $(\boldsymbol{f}^{a(c)}, \boldsymbol{\tau}^{a(c)})$, and $(\boldsymbol{f}^{a(s)}, \boldsymbol{\tau}^{a(s)})$ denote viscous, conservative, and stochastic loads. Here all loads for body a are referred to the reference point $\boldsymbol{r}^a$. We assume that the viscous loads are of the general linear form

$$\boldsymbol{f}^{a(v)} = -\sum_{b=1}^{n}\Big(\boldsymbol{\gamma}_1^{ab}\boldsymbol{v}^b + \boldsymbol{\gamma}_3^{ab}\boldsymbol{\omega}^b\Big), \qquad \boldsymbol{\tau}^{a(v)} = -\sum_{b=1}^{n}\Big(\boldsymbol{\gamma}_2^{ab}\boldsymbol{v}^b + \boldsymbol{\gamma}_4^{ab}\boldsymbol{\omega}^b\Big), \tag{5.5}$$

where $\boldsymbol{\gamma}_1^{ab}, \dots, \boldsymbol{\gamma}_4^{ab}$ $(a, b = 1, \dots, n)$ are given tensors which in general may depend on the configuration of the system. We suppose that the conservative loads $(\boldsymbol{f}^{a(c)}, \boldsymbol{\tau}^{a(c)})$ satisfy, for all possible motions of the system,

$$\sum_{b=1}^{n}\Big(\boldsymbol{f}^{b(c)} \cdot \boldsymbol{v}^b + \boldsymbol{\tau}^{b(c)} \cdot \boldsymbol{\omega}^b\Big) = -\dot{U}, \tag{5.6}$$

where U is a prescribed potential energy function. Last, we assume that the stochastic loads $(\boldsymbol{f}^{a(s)}, \boldsymbol{\tau}^{a(s)})$ are white-noise-type loads of the form

$$\boldsymbol{f}^{a(s)} = \sum_{b=1}^{n}\Big(\boldsymbol{\sigma}_1^{ab}\dot{\boldsymbol{W}}^{b,\mathrm{lin}} + \boldsymbol{\sigma}_3^{ab}\dot{\boldsymbol{W}}^{b,\mathrm{ang}}\Big), \quad \boldsymbol{\tau}^{a(s)} = \sum_{b=1}^{n}\Big(\boldsymbol{\sigma}_2^{ab}\dot{\boldsymbol{W}}^{b,\mathrm{lin}} + \boldsymbol{\sigma}_4^{ab}\dot{\boldsymbol{W}}^{b,\mathrm{ang}}\Big), \tag{5.7}$$

where $\boldsymbol{\sigma}_1^{ab}, \dots, \boldsymbol{\sigma}_4^{ab}$ are given tensors which in general may depend on the configuration of the system and $(\boldsymbol{W}^{b,\mathrm{lin}}, \boldsymbol{W}^{b,\mathrm{ang}})$ denote standard, independent Wiener processes $(a, b = 1, \dots, n)$. As before, the form of these loads is motivated by (5.5).

5.3. Euler–Langevin equations, components. Substituting (5.4), (5.5), and (5.7) into (5.3), combining the result with (5.1), and using the antisymmetry of the vector product, we obtain the Euler–Langevin equations of motion for each body a, namely

$$
\begin{aligned}
\dot{\boldsymbol{r}}^a &= \boldsymbol{v}^a,\\
\dot{\boldsymbol{d}}_i^a &= \boldsymbol{\omega}^a \times \boldsymbol{d}_i^a,\\
\dot{\boldsymbol{p}}^a &= \boldsymbol{f}^{a(c)} - \sum_{b=1}^n \big(\boldsymbol{\gamma}_1^{ab}\boldsymbol{v}^b + \boldsymbol{\gamma}_3^{ab}\boldsymbol{\omega}^b\big) + \sum_{b=1}^n \big(\boldsymbol{\sigma}_1^{ab}\dot{\boldsymbol{W}}^{b,\mathrm{lin}} + \boldsymbol{\sigma}_3^{ab}\dot{\boldsymbol{W}}^{b,\mathrm{ang}}\big),\\
\dot{\boldsymbol{\pi}}^a &= \boldsymbol{p}^a \times (\boldsymbol{c}^a \times \boldsymbol{\omega}^a) + \boldsymbol{\tau}^{a(c)} - \sum_{b=1}^n \big(\boldsymbol{\gamma}_2^{ab}\boldsymbol{v}^b + \boldsymbol{\gamma}_4^{ab}\boldsymbol{\omega}^b\big)\\
&\qquad + \sum_{b=1}^n \big(\boldsymbol{\sigma}_2^{ab}\dot{\boldsymbol{W}}^{b,\mathrm{lin}} + \boldsymbol{\sigma}_4^{ab}\dot{\boldsymbol{W}}^{b,\mathrm{ang}}\big),
\end{aligned}
\tag{5.8}
$$

where $\boldsymbol{p}^a = m^a(\boldsymbol{v}^a + \boldsymbol{\omega}^a \times \boldsymbol{c}^a)$ and $\boldsymbol{\pi}^a = \boldsymbol{I}^a\boldsymbol{\omega}^a + \boldsymbol{c}^a \times \boldsymbol{p}^a$. Notice that the equations for all $a = 1, \dots, n$ are coupled through the assumed form of the resultant loads.

As before, we can express (5.8) in terms of a convenient set of components. Let $Q^a \in SO_3 \subset \mathbb{R}^{3\times 3}$ denote the component matrix of the body frame $\{\boldsymbol{d}_i^a\}$ in the fixed frame $\{\boldsymbol{e}_i\}$, that is, $Q_{ij}^a = \boldsymbol{e}_i \cdot \boldsymbol{d}_j^a$. Moreover, let $v^a \in \mathbb{R}^3$, $I^a \in \mathbb{R}^{3\times 3}$, and so on denote component vectors and matrices in the frame $\{\boldsymbol{d}_i^a\}$, that is, $v_i^a = \boldsymbol{d}_i^a \cdot \boldsymbol{v}^a$, $I_{ij}^a = \boldsymbol{d}_i^a \cdot \boldsymbol{I}^a\boldsymbol{d}_j^a$, and so on. Furthermore, let $\gamma_1^{ab} \in \mathbb{R}^{3\times 3}$, $\sigma_1^{ab} \in \mathbb{R}^{3\times 3}$, and so on denote component matrices with respect to the pair $\{\boldsymbol{d}_i^a\}$ and $\{\boldsymbol{d}_i^b\}$, that is, $(\gamma_1^{ab})_{ij} = \boldsymbol{d}_i^a \cdot \boldsymbol{\gamma}_1^{ab}\boldsymbol{d}_j^b$, $(\sigma_1^{ab})_{ij} = \boldsymbol{d}_i^a \cdot \boldsymbol{\sigma}_1^{ab}\boldsymbol{d}_j^b$, and so on. Then by straightforward calculation as before we find that the equations in (5.8) for each body a become

$$
\begin{aligned}
\dot{r}^a &= r^a \times \omega^a + v^a,\\
\dot{Q}^a &= Q^a[\omega^a\times],\\
\dot{p}^a &= p^a \times \omega^a + f^{a(c)} - \sum_{b=1}^n \big(\gamma_1^{ab}v^b + \gamma_3^{ab}\omega^b\big)\\
&\qquad + \sum_{b=1}^n \big(\sigma_1^{ab}\dot{W}^{b,\mathrm{lin}} + \sigma_3^{ab}\dot{W}^{b,\mathrm{ang}}\big),\\
\dot{\pi}^a &= \pi^a \times \omega^a + p^a \times (c^a \times \omega^a) + \tau^{a(c)} - \sum_{b=1}^n \big(\gamma_2^{ab}v^b + \gamma_4^{ab}\omega^b\big)\\
&\qquad + \sum_{b=1}^n \big(\sigma_2^{ab}\dot{W}^{b,\mathrm{lin}} + \sigma_4^{ab}\dot{W}^{b,\mathrm{ang}}\big),
\end{aligned}
\tag{5.9}
$$

where $p^a = m^a(v^a + \omega^a \times c^a)$, $\pi^a = I^a\omega^a + c^a \times p^a$, and $[\omega^a\times] \in \mathbb{R}^{3\times 3}$ denotes the skew-symmetric matrix defined in (2.13).

We interpret (5.9) as a coupled system of stochastic differential equations in the sense of Itô for the phase variables $(r^a, Q^a, p^a, \pi^a)_{a=1}^n$ which evolve in the space $[\mathbb{R}^3 \times SO_3 \times \mathbb{R}^3 \times \mathbb{R}^3]^n$. In this system, the scalars m^a, the component vectors c^a, and the component matrices I^a are all assumed to be constant. The component matrices $\gamma_1^{ab}, \dots, \gamma_4^{ab}$ and $\sigma_1^{ab}, \dots, \sigma_4^{ab}$ and the function U appearing in (5.5), (5.6), and (5.7) are all assumed to be functions of all the configuration variables $(r^a, Q^a)_{a=1}^n$. Indeed, the potential energy function U may model both local and nonlocal interactions in the system.

5.4. Hamilton–Langevin formulation, measures. The results in sections 3 and 4 can be extended in a straightforward way to a system of bodies. To this end, let

$x = (x^a)_{a=1}^n \in \mathbb{R}^{6n}$, $\nu = (\nu^a)_{a=1}^n \in \mathbb{R}^{6n}$, and $y = (y^a)_{a=1}^n \in \mathbb{R}^{6n}$, where $x^a = (r^a, \eta^a)$ are the configuration coordinates, $\nu^a = (v^a, \omega^a)$ are the velocity components, and $y^a = (\psi^a, \zeta^a)$ are the canonical momenta for body a. Moreover, let $G = \mathrm{diag}(G^a)_{a=1}^n \in \mathbb{R}^{6n\times 6n}$ and $M = \mathrm{diag}(M^a)_{a=1}^n \in \mathbb{R}^{6n\times 6n}$, where G^a is the velocity structure matrix for body a defined such that $\nu^a = G^a \dot{x}^a$ and M^a is the mass matrix for body a. Furthermore, let $\gamma = (\gamma^{ab})_{a,b=1}^n \in \mathbb{R}^{6n\times 6n}$, $\sigma = (\sigma^{ab})_{a,b=1}^n \in \mathbb{R}^{6n\times 6n}$, and $W = (W^b)_{b=1}^n \in \mathbb{R}^{6n}$, where γ^{ab}, σ^{ab}, and W^b are defined by

$$\gamma^{ab} = \begin{pmatrix} \gamma_1^{ab} & \gamma_3^{ab} \\ \gamma_2^{ab} & \gamma_4^{ab} \end{pmatrix}, \qquad \sigma^{ab} = \begin{pmatrix} \sigma_1^{ab} & \sigma_3^{ab} \\ \sigma_2^{ab} & \sigma_4^{ab} \end{pmatrix}, \qquad W^b = \begin{pmatrix} W^{b,\mathrm{lin}} \\ W^{b,\mathrm{ang}} \end{pmatrix}. \tag{5.10}$$

Using the notation outlined above, it can now be seen that all results in sections 3 and 4 pertaining to the Hamiltonian form of the equations of motion and the associated canonical measures on phase, configuration, and velocity space can be extended to a system of bodies. In particular, just as in Proposition 3.6, we find that the equations of motion (5.9) can be written in the canonical Hamiltonian form

$$\begin{aligned} \dot{x} &= \frac{\partial H}{\partial y}, \qquad \dot{y} = -\frac{\partial H}{\partial x} - G^T\gamma G\frac{\partial H}{\partial y} + G^T\sigma\dot{W}, \\ H(x,y) &= \frac{1}{2} y \cdot G^{-1}M^{-1}G^{-T}y + U(x). \end{aligned} \tag{5.11}$$

As in Proposition 3.7, these equations are invariant under a change of variables of the form (3.64). Moreover, under the same conditions as in Proposition 4.1, the canonical measure

$$\mu(dx, dy) = \frac{1}{C} e^{-\beta H(x,y)}\, dx\, dy, \tag{5.12}$$

where $\beta = 1/(\kappa\Theta)$ and C are positive constants, is a stationary measure for (5.11). Also, as in Proposition 4.2, this measure is invariant under a change of variables of the form (3.64). Furthermore, for arbitrary potential energy $U(x)$ and kinetic energy $\Phi(\nu) = \frac{1}{2}\nu \cdot M\nu$, we find, just as in Proposition 4.3, that the canonical measure μ is equivalent to the product of a canonical configuration measure μ^{con} and a velocity measure μ^{vel} defined as

$$\mu^{\mathrm{con}}(dx) = \frac{1}{C'} e^{-\beta U(x)} |G(x)|\, dx, \qquad \mu^{\mathrm{vel}}(d\nu) = \frac{1}{C''} e^{-\beta\Phi(\nu)}\, d\nu, \tag{5.13}$$

where C' and C'' are positive constants and $|G(x)|$ denotes the determinant of the velocity structure matrix $G(x)$. As in Proposition 4.4, the canonical configuration measure is invariant under an arbitrary change of configuration variables, and so too is the velocity measure by virtue of its definition.

6. General quadratic models. Here we specialize the results from section 5 to a rigid body model of a topologically linear polymer. We consider the case in which the potential energy of the system is a general quadratic function of a natural set of internal coordinates describing the relative, three-dimensional displacements and rotations between bodies. We outline the internal coordinates for this system and derive explicit forms for the associated canonical measures on the various spaces. Furthermore, we characterize the complete set of potential energy and mass parameters of the model in terms of ratios of certain expected values.

6.1. Internal coordinates. Consider a model of a topologically linear polymer in which each monomer unit is modeled as an independent rigid body with reference point $\boldsymbol{r}^a$ and body frame $\{\boldsymbol{d}_i^a\}$ $(a = 1, \ldots, n)$. Then the relative displacement and rotation between bodies a and $a+1$ along the polymer are completely described by a coordinate vector $\xi^a \in \mathbb{R}^3$ and a rotation matrix $L^a \in SO_3$ such that

$$\boldsymbol{r}^{a+1} = \boldsymbol{r}^a + \xi_i^a \boldsymbol{h}_i^{a,a+1}, \qquad \boldsymbol{d}_j^{a+1} = L_{ij}^a \boldsymbol{d}_i^a, \tag{6.1}$$

where $\{\boldsymbol{h}_i^{a,a+1}\}$ is a right-handed, orthonormal frame that depends on $\{\boldsymbol{d}_i^a\}$ and $\{\boldsymbol{d}_i^{a+1}\}$. The coordinate vector ξ^a describes the position of $\boldsymbol{r}^{a+1}$ with respect to $\boldsymbol{r}^a$ in the frame $\{\boldsymbol{h}_i^{a,a+1}\}$. In applications to DNA, the frame $\{\boldsymbol{h}_i^{a,a+1}\}$ is typically chosen as an average of $\{\boldsymbol{d}_i^a\}$ and $\{\boldsymbol{d}_i^{a+1}\}$. The rotation matrix L^a describes the orientation of frame $\{\boldsymbol{d}_i^{a+1}\}$ with respect to $\{\boldsymbol{d}_i^a\}$. Throughout our developments, we suppose that each $L^a \in SO_3$ is parameterized by local coordinates $\theta^a \in \mathcal{A} \subset \mathbb{R}^3$ with angular velocity structure matrix $S(\theta^a) \in \mathbb{R}^{3\times 3}$.

From (6.1) we deduce that the entries in ξ^a and L^a are given by

$$\xi_i^a = \boldsymbol{h}_i^{a,a+1} \cdot (\boldsymbol{r}^{a+1} - \boldsymbol{r}^a), \qquad L_{ij}^a = \boldsymbol{d}_i^a \cdot \boldsymbol{d}_j^{a+1}. \tag{6.2}$$

Let $P^{a,a+1} \in SO_3$ denote the component matrix of the frame $\{\boldsymbol{h}_i^{a,a+1}\}$ in the fixed frame $\{\boldsymbol{e}_i\}$, that is, $P_{ij}^{a,a+1} = \boldsymbol{e}_i \cdot \boldsymbol{h}_j^{a,a+1}$. Then, using the facts that $\boldsymbol{d}_i^a = Q_{ki}^a \boldsymbol{e}_k$, $\boldsymbol{r}^a = r_i^a \boldsymbol{d}_i^a$, $\boldsymbol{d}_i^{a+1} = Q_{ki}^{a+1} \boldsymbol{e}_k$, and $\boldsymbol{r}^{a+1} = r_i^{a+1} \boldsymbol{d}_i^{a+1}$, we deduce that (6.2) can be written in the matrix form

$$\xi^a = \big(P^{a,a+1}\big)^T \big(Q^{a+1} r^{a+1} - Q^a r^a\big), \qquad L^a = \big(Q^a\big)^T Q^{a+1}. \tag{6.3}$$

As with the matrices L^a, we suppose that each $Q^a \in SO_3$ is parameterized by local coordinates $\eta^a \in \mathcal{A} \subset \mathbb{R}^3$ with angular velocity structure matrix $S(\eta^a) \in \mathbb{R}^{3\times 3}$.

The relative displacement and rotation coordinates (ξ^a, θ^a) $(a = 1, \ldots, n-1)$ describe the configuration of the system up to an overall translation and rotation. To complete the specification of the configuration we introduce a coordinate vector ξ^0 and a rotation matrix L^0, with coordinates θ^0, such that

$$\boldsymbol{r}^1 = \boldsymbol{r}^0 + \xi_i^0 \boldsymbol{d}_i^0, \qquad \boldsymbol{d}_j^1 = L_{ij}^0 \boldsymbol{d}_i^0, \tag{6.4}$$

where $\boldsymbol{r}^0$ is a lab-fixed reference point and $\{\boldsymbol{d}_i^0\}$ is a lab-fixed frame, which without loss of generality we identify with $\mathbf{0}$ and $\{\boldsymbol{e}_i\}$, respectively. With this convention, we find that the coordinate vector ξ^0 and the rotation matrix L^0 are given by

$$\xi^0 = Q^1 r^1, \qquad L^0 = Q^1. \tag{6.5}$$

Thus the configuration of the system is completely described by the coordinates $q^a = (\xi^a, \theta^a) \in \mathbb{R}^6$ $(a = 0, \ldots, n-1)$. Notice that q^0 are external coordinates that specify the spatial location of the polymer, whereas $q^1, \ldots, q^{n-1}$ are internal coordinates that describe its shape. In the terminology of mechanics, the internal coordinates ξ^a would be referred to as shear and extension strains and θ^a as bending and twisting strains. In applications to DNA, ξ^a would be referred to as shift-slide-rise coordinates and θ^a as tilt-roll-twist coordinates between bodies a and $a+1$.

6.2. Jacobian for internal coordinates. Consider the change of variables from (η^a, r^a) $(a = 1 \ldots, n)$ to (θ^a, ξ^a) $(a = 0 \ldots, n-1)$ defined by (6.3) and (6.5),

where for convenience we have reordered the variables. This change of variables is of the form

$$\begin{array}{rcll} \theta^0 &=& \theta^0(\eta^1), & \\ \theta^a &=& \theta^a(\eta^a, \eta^{a+1}) & (a = 1, \dots, n-1), \\ \xi^0 &=& \xi^0(\eta^1, r^1), & \\ \xi^a &=& \xi^a(\eta^a, \eta^{a+1}, r^a, r^{a+1}) & (a = 1, \dots, n-1). \end{array} \tag{6.6}$$

Using the notation $\theta = (\theta^0, \dots, \theta^{n-1})$, $\eta = (\eta^1, \dots, \eta^n)$, and so on, we notice that the Jacobian matrix

$$\frac{\partial(\theta, \xi)}{\partial(\eta, r)} = \left(\begin{array}{ccc|ccc} \frac{\partial\theta^0}{\partial\eta^1} & \cdots & \frac{\partial\theta^0}{\partial\eta^n} & \frac{\partial\theta^0}{\partial r^1} & \cdots & \frac{\partial\theta^0}{\partial r^n} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial\theta^{n-1}}{\partial\eta^1} & \cdots & \frac{\partial\theta^{n-1}}{\partial\eta^n} & \frac{\partial\theta^{n-1}}{\partial r^1} & \cdots & \frac{\partial\theta^{n-1}}{\partial r^n} \\ \hline \frac{\partial\xi^0}{\partial\eta^1} & \cdots & \frac{\partial\xi^0}{\partial\eta^n} & \frac{\partial\xi^0}{\partial r^1} & \cdots & \frac{\partial\xi^0}{\partial r^n} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial\xi^{n-1}}{\partial\eta^1} & \cdots & \frac{\partial\xi^{n-1}}{\partial\eta^n} & \frac{\partial\xi^{n-1}}{\partial r^1} & \cdots & \frac{\partial\xi^{n-1}}{\partial r^n} \end{array}\right) \tag{6.7}$$

is in fact lower triangular for changes of variables of the form (6.6). Since the magnitude of a determinant is invariant under reorderings of its columns and rows, we deduce that the change of variables from $x = (x^1, \dots, x^n)$ to $q = (q^0, \dots, q^{n-1})$, where $x^a = (r^a, \eta^a)$ and $q^a = (\xi^a, \theta^a)$, has Jacobian determinant

$$\left|\frac{\partial q}{\partial x}\right| = \prod_{a=0}^{n-1} \left|\frac{\partial\theta^a}{\partial\eta^{a+1}}\right| \left|\frac{\partial\xi^a}{\partial r^{a+1}}\right|. \tag{6.8}$$

The above determinant can be characterized explicitly. From (6.3) and (6.5) we deduce that the derivative $\partial\xi^a/\partial r^{a+1}$ is an orthogonal matrix for all a, which implies $|\partial\xi^a/\partial r^{a+1}| = 1$ for all a. To derive an expression for the derivative $\partial\theta^a/\partial\eta^{a+1}$, we consider an arbitrary curve $\alpha \mapsto \eta^{a+1}(\alpha)$. Then from (6.6) we have $\theta^a(\alpha) = \theta^a(\eta^a, \eta^{a+1}(\alpha))$, and by the chain rule we get, using a circle to denote the derivative with respect to α,

$$\mathring{\theta}^a = \left(\frac{\partial\theta^a}{\partial\eta^{a+1}}\right) \mathring{\eta}^{a+1}. \tag{6.9}$$

Moreover, from (6.3) we have $L^a(\alpha) = (Q^a)^T Q^{a+1}(\alpha)$. Differentiating this relation and using Proposition 3.1(i), we get

$$\begin{array}{rcl} \mathring{L}^a &=& (Q^a)^T \mathring{Q}^{a+1}, \\ L^a\big[\big(S(\theta^a)\mathring{\theta}^a\big)\times\big] &=& (Q^a)^T Q^{a+1}\big[\big(S(\eta^{a+1})\mathring{\eta}^{a+1}\big)\times\big], \\ S(\theta^a)\mathring{\theta}^a &=& S(\eta^{a+1})\mathring{\eta}^{a+1}, \\ \mathring{\theta}^a &=& S(\theta^a)^{-1} S(\eta^{a+1})\mathring{\eta}^{a+1}. \end{array} \tag{6.10}$$

Comparing (6.10) and (6.9) we find $\partial\theta^a/\partial\eta^{a+1} = S(\theta^a)^{-1}S(\eta^{a+1})$, which can be shown to hold for all a. Substitution of this result into (6.8) gives

$$\left|\frac{\partial q}{\partial x}\right| = \prod_{a=0}^{n-1} \big|S(\theta^a)\big|^{-1} \big|S(\eta^{a+1})\big|. \tag{6.11}$$

6.3. Configuration and velocity measures. For arbitrary potential energy $U(x)$ and kinetic energy $\Phi(\nu)$, the behavior of the polymer model in thermal equilibrium is described by the canonical configuration measure μ^{con} and the velocity measure μ^{vel}, where

$$\mu^{\mathrm{con}}(dx) = \frac{1}{C'} e^{-\beta U(x)} |G(x)|\, dx, \qquad \mu^{\mathrm{vel}}(d\nu) = \frac{1}{C''} e^{-\beta \Phi(\nu)}\, d\nu. \tag{6.12}$$

In view of (6.11), the measure μ^{con} on the absolute configuration coordinates x can be transformed into an equivalent measure $\mu^{\mathrm{con}}_{\mathrm{rel}}$ on the relative configuration coordinates q, namely

$$\mu^{\mathrm{con}}_{\mathrm{rel}}(dq) = \frac{1}{C'} e^{-\beta U(x(q))} \mathcal{J}(q)\, dq, \quad \text{where} \quad \mathcal{J}(q) = \big|G(x(q))\big| \left|\frac{\partial x}{\partial q}\right|. \tag{6.13}$$

Using the fact that $G = \mathrm{diag}(G^a)_{a=1}^n$, together with (3.24) and (6.11), we deduce that the Jacobian factor $\mathcal{J}(q)$ is given by

$$\mathcal{J}(q) = \prod_{a=0}^{n-1} \big|S(\theta^a)\big|. \tag{6.14}$$

Assuming a decomposition $U(x(q)) = U_{\mathrm{ext}}(q^0) + U_{\mathrm{int}}(q^1, \ldots, q^{n-1})$, where U_{ext} and U_{int} are external and internal potential energy functions, the measure $\mu^{\mathrm{con}}_{\mathrm{rel}}$ can be factored into a measure $\mu^{\mathrm{con}}_{\mathrm{ext}}$ on the external coordinate q^0 and a measure $\mu^{\mathrm{con}}_{\mathrm{int}}$ on the internal coordinates $w = (q^1, \ldots, q^{n-1})$. In particular, we have $\mu^{\mathrm{con}}_{\mathrm{rel}} = \mu^{\mathrm{con}}_{\mathrm{ext}} \mu^{\mathrm{con}}_{\mathrm{int}}$, where

$$\mu^{\mathrm{con}}_{\mathrm{ext}}(dq^0) = \frac{1}{C'_{\mathrm{ext}}} e^{-\beta U_{\mathrm{ext}}(q^0)} \mathcal{J}_{\mathrm{ext}}(q^0)\, dq^0, \qquad \mu^{\mathrm{con}}_{\mathrm{int}}(dw) = \frac{1}{C'_{\mathrm{int}}} e^{-\beta U_{\mathrm{int}}(w)} \mathcal{J}_{\mathrm{int}}(w)\, dw. \tag{6.15}$$

Here C'_{ext} and C'_{int} are positive constants, and $\mathcal{J}_{\mathrm{ext}}(q^0)$ and $\mathcal{J}_{\mathrm{int}}(w)$ are Jacobian factors given by

$$\mathcal{J}_{\mathrm{ext}}(q^0) = \big|S(\theta^0)\big|, \qquad \mathcal{J}_{\mathrm{int}}(w) = \prod_{a=1}^{n-1} \big|S(\theta^a)\big|. \tag{6.16}$$

The above result shows that, for a system in thermal equilibrium, the configuration and velocity variables q^0, w, and ν are distributed according to the independent measures $\mu^{\mathrm{con}}_{\mathrm{ext}}$, $\mu^{\mathrm{con}}_{\mathrm{int}}$, and μ^{vel}. That is, q^0, w, and ν are statistically independent. As a consequence, the expected or average value of any functions $f(q^0)$, $g(w)$, and $h(\nu)$ is given by

$$\begin{aligned} \mathbb{E}_{\mu^{\mathrm{con}}_{\mathrm{ext}}}[f] &= \int_{\mathcal{X}_{\mathrm{ext}}} f(q^0)\, \mu^{\mathrm{con}}_{\mathrm{ext}}(dq^0), \\ \mathbb{E}_{\mu^{\mathrm{con}}_{\mathrm{int}}}[g] = \int_{\mathcal{X}_{\mathrm{int}}} g(w)\, \mu^{\mathrm{con}}_{\mathrm{int}}(dw), &\qquad \mathbb{E}_{\mu^{\mathrm{vel}}}[h] = \int_{\mathcal{V}} h(\nu)\, \mu^{\mathrm{vel}}(d\nu). \end{aligned} \tag{6.17}$$

Here $\mathcal{X}_{\mathrm{ext}} \subset \mathbb{R}^6$ is a prescribed domain for q^0, $\mathcal{X}_{\mathrm{int}} \subset \mathbb{R}^{6n-6}$ is a prescribed domain for w, and $\mathcal{V} = \mathbb{R}^{6n}$ is the domain for ν. Assuming all measures are normalizable we have

$$\begin{aligned} \mathbb{E}_{\mu^{\mathrm{con}}_{\mathrm{ext}}}[f] &= \frac{\int_{\mathcal{X}_{\mathrm{ext}}} e^{-\beta U_{\mathrm{ext}}(q^0)} f(q^0) \mathcal{J}_{\mathrm{ext}}(q^0)\, dq^0}{\int_{\mathcal{X}_{\mathrm{ext}}} e^{-\beta U_{\mathrm{ext}}(q^0)} \mathcal{J}_{\mathrm{ext}}(q^0)\, dq^0}, \\ \mathbb{E}_{\mu^{\mathrm{con}}_{\mathrm{int}}}[g] = \frac{\int_{\mathcal{X}_{\mathrm{int}}} e^{-\beta U_{\mathrm{int}}(w)} g(w) \mathcal{J}_{\mathrm{int}}(w)\, dw}{\int_{\mathcal{X}_{\mathrm{int}}} e^{-\beta U_{\mathrm{int}}(w)} \mathcal{J}_{\mathrm{int}}(w)\, dw}, &\qquad \mathbb{E}_{\mu^{\mathrm{vel}}}[h] = \frac{\int_{\mathcal{V}} e^{-\beta \Phi(\nu)} h(\nu)\, d\nu}{\int_{\mathcal{V}} e^{-\beta \Phi(\nu)}\, d\nu}. \end{aligned} \tag{6.18}$$

From the relations in (6.18) we observe that the expected value of an arbitrary function $h(\nu)$ is entirely dependent on the kinetic energy $\Phi(\nu)$. In contrast, the expected value of an arbitrary function $g(w)$ is not entirely dependent on the internal potential energy $U_{\text{int}}(w)$; it also depends on the Jacobian factor $\mathcal{J}_{\text{int}}(w)$. However, a quantity that is entirely dependent on $U_{\text{int}}(w)$ is given by the ratio

$$\frac{\mathbb{E}_{\mu_{\text{int}}^{\text{con}}}[g/\mathcal{J}_{\text{int}}]}{\mathbb{E}_{\mu_{\text{int}}^{\text{con}}}[1/\mathcal{J}_{\text{int}}]} = \frac{\int_{\mathcal{X}_{\text{int}}} e^{-\beta U_{\text{int}}(w)} g(w)\, dw}{\int_{\mathcal{X}_{\text{int}}} e^{-\beta U_{\text{int}}(w)}\, dw}. \tag{6.19}$$

These observations will be exploited below to characterize the material parameters associated with $U_{\text{int}}(w)$ and $\Phi(\nu)$.

6.4. Quadratic energy model. For a polymer model with n bodies we consider an internal potential energy function of the general quadratic form

$$U_{\text{int}}(w) = \frac{1}{2}(w - \widehat{w}) \cdot K(w - \widehat{w}), \tag{6.20}$$

where the vector $\widehat{w} = (\widehat{q}^1, \ldots, \widehat{q}^{n-1}) \in \mathbb{R}^{6n-6}$ and the symmetric, positive-definite matrix $K \in \mathbb{R}^{(6n-6)\times(6n-6)}$ are material parameters. The vector $\widehat{w}$ corresponds to the equilibrium or ground-state value of w. In particular, $\widehat{q}^a$ is the equilibrium value of the relative displacement and rotation coordinates q^a between bodies a and $a+1$. The matrix K is referred to as the stiffness matrix. It provides a measure of the elastic stiffness associated with each of the internal coordinates and couplings between them, and need not be assumed to be block-diagonal.

As outlined in section 5, the kinetic energy of a system of n bodies is given by

$$\Phi(\nu) = \frac{1}{2}\nu \cdot M\nu, \tag{6.21}$$

where $M = \text{diag}(M^1, \ldots, M^n) \in \mathbb{R}^{6n\times 6n}$ is a symmetric, positive-definite matrix of mass parameters. In particular, each M^a is the mass matrix for body a as defined in (3.27). In our developments below, we use the notation $w \otimes w$ and $\nu \otimes \nu$ to denote the usual outer or matrix product of the vectors w and ν. Thus $[w \otimes w]_{pq} = w_p w_q$ and $[\nu \otimes \nu]_{pq} = \nu_p \nu_q$.

The relations in (6.18) and (6.19) can be exploited to derive explicit characterizations of the parameters $\widehat{w}$, K, and M. Notice that, although the internal potential energy U_{int} is quadratic, the measure $\mu_{\text{int}}^{\text{con}}$ is non-Gaussian due to the presence of the Jacobian factor $\mathcal{J}_{\text{int}}$. As a result, the parameters $\widehat{w}$ and K are not given by the usual moment relations for Gaussian measures. However, from (6.19) we see that $\widehat{w}$ can be characterized as a ratio of expected values. In particular, substituting the vector-valued function $g(w) = w$ into (6.19) and assuming $\mathcal{X}_{\text{int}} = \mathbb{R}^{6n-6}$, we obtain, by standard results for Gaussian integrals,

$$\widehat{w} = \frac{\int_{\mathcal{X}_{\text{int}}} e^{-\beta U_{\text{int}}(w)} w\, dw}{\int_{\mathcal{X}_{\text{int}}} e^{-\beta U_{\text{int}}(w)}\, dw} = \frac{\mathbb{E}_{\mu_{\text{int}}^{\text{con}}}[w/\mathcal{J}_{\text{int}}]}{\mathbb{E}_{\mu_{\text{int}}^{\text{con}}}[1/\mathcal{J}_{\text{int}}]}. \tag{6.22}$$

Thus $\widehat{w}$ is not equal to the expected value of w but rather to a ratio of expected values which are weighted by the Jacobian $\mathcal{J}_{\text{int}}(w)$.

The stiffness matrix K can also be characterized similarly. Substituting the matrix-valued function $g(w) = \Delta w \otimes \Delta w$ into (6.19), where $\Delta w = w - \widehat{w}$, we get,

again assuming $\mathcal{X}_{\text{int}} = \mathbb{R}^{6n-6}$ and using standard results for Gaussian integrals,

$$\frac{1}{\beta}K^{-1} = \frac{\int_{\mathcal{X}_{\text{int}}} e^{-\beta U_{\text{int}}(w)} \Delta w \otimes \Delta w \, dw}{\int_{\mathcal{X}_{\text{int}}} e^{-\beta U_{\text{int}}(w)} \, dw} = \frac{\mathbb{E}_{\mu_{\text{int}}^{\text{con}}}[\Delta w \otimes \Delta w / \mathcal{J}_{\text{int}}]}{\mathbb{E}_{\mu_{\text{int}}^{\text{con}}}[1/\mathcal{J}_{\text{int}}]}. \tag{6.23}$$

Thus, just as with $\widehat{w}$, the matrix $\frac{1}{\beta}K^{-1}$ is not equal to the expected value of $\Delta w \otimes \Delta w$ but rather to a ratio of weighted expected values. By expanding the right-hand side of (6.23) and using (6.22), we deduce that

$$\frac{1}{\beta}K^{-1} + \widehat{w} \otimes \widehat{w} = \frac{\mathbb{E}_{\mu_{\text{int}}^{\text{con}}}[w \otimes w / \mathcal{J}_{\text{int}}]}{\mathbb{E}_{\mu_{\text{int}}^{\text{con}}}[1/\mathcal{J}_{\text{int}}]}, \tag{6.24}$$

which may be more convenient than (6.23) since the expected values on the right-hand side of (6.24) are purely kinematic and independent of the model parameters $\widehat{w}$.

The characterization of the mass matrix M is simpler due to the Gaussian form of the measure μ^{vel}. In particular, substituting the matrix-valued function $h(\nu) = \nu \otimes \nu$ into (6.18) and using standard results for Gaussian integrals, we get

$$\frac{1}{\beta}M^{-1} = \frac{\int_{\mathcal{V}} e^{-\beta \Phi(\nu)} \nu \otimes \nu \, d\nu}{\int_{\mathcal{V}} e^{-\beta \Phi(\nu)} \, d\nu} = \mathbb{E}_{\mu^{\text{vel}}}[\nu \otimes \nu]. \tag{6.25}$$

Thus the matrix $\frac{1}{\beta}M^{-1}$ is equal to the expected value of $\nu \otimes \nu$. Moreover, since $M = \text{diag}(M^1, \ldots, M^n)$, we have $M^{-1} = \text{diag}([M^1]^{-1}, \ldots, [M^n]^{-1})$, where M^a and $[M^a]^{-1}$ are explicit functions of the mass parameters of body a as defined in (3.27).

7. Summary. We have developed properly invariant formulations of the inertial dynamics of a system of rigid bodies interacting both with each other, through a potential dependent upon relative location and orientation, and with a solvent, modeled implicitly by viscous and stochastic forcing terms. Our analysis demonstrates that the invariance properties arise because, whenever the usual chain rule of deterministic calculus is, as it must be in the stochastic context, replaced with the more complicated Itô formula, the classic invariances nevertheless persist. The governing equations express the balance laws of linear and angular momenta of each body and allow a full coupling between the translational and rotational degrees of freedom of all bodies. These are the equations that we refer to as Euler–Langevin.

We studied the classic canonical measure for the Euler–Langevin model and examined the implications of different choices of coordinates. The hypotheses of the fluctuation-dissipation theorem, specifically those pertaining to normalizability and boundaries, which provide conditions for the canonical measure to be stationary, or equivalently for the system to be in thermal equilibrium, were shown to impose different restrictions on the system potential energy depending on the type of rotational coordinate chart. The restrictions suggest that Cayley-type charts are appropriate for systems with strongly restrained rotational degrees of freedom, whereas Euler-type charts are appropriate for systems with unrestrained rotational degrees of freedom. We also studied the factorability of the canonical measure and showed that, by a change of variables on the momenta, the measure can always be explicitly factored into independent, properly invariant canonical measures on the configuration and body velocity spaces, the former of which contains a Jacobian factor associated with the three-dimensional rotation group.

We believe the Euler–Langevin equations to be an appropriate coarse-grained model of a polymer at mesoscales in which monomer units can be approximated as

rigid and the effects of a solvent can be approximated by implicit terms. We have a particular interest in the development of coarse-grained models of stiff, linear polymers such as DNA, where the appropriate and biologically important mesoscales are a few tens to a few hundreds of basepairs. At these scales, inhomogeneous effects dependent upon the specific basepair sequence, and the relative orientations of individual basepairs, can be significant. The model outlined here can capture this level of detail at these scales, which distinguishes it from other more standard models of polymer physics, such as chain-type models based on bead or link elements. Indeed, whereas other more standard models have proven to be very successful at longer length scales, they are typically homogeneous and typically neglect some or all rotational degrees of freedom of the individual elements, which may be overly idealistic at the mesoscales of interest here.

We have shown that, for the important case of a linear polymer, the Euler–Langevin model can be understood and parameterized in simple physical terms. Each rigid body can be taken as a model for an individual monomer unit, and the internal junction coordinates provide a direct, complete, and independent measure of the relative, three-dimensional displacement and rotation between adjacent units. In the quadratic approximation, the potential energy can be parameterized by the ground-state values of these junction coordinates, along with a symmetric, positive-definite elastic stiffness matrix associated with deformations from the ground state. While the linearity of the polymer guarantees that the degrees of freedom at each junction are independent in the sense of there being no kinematic constraint between them, it is nevertheless perfectly possible that the stiffness matrix might not be block-diagonal; that is, there could be forces and moments of interaction between nonadjacent monomer units. In contrast, the kinetic energy is parameterized by standard mass and inertia parameters associated with each individual monomer unit, leading to a block-diagonal generalized mass matrix for the system, which is also necessarily symmetric and positive-definite.

We have also shown that, under the assumption of thermal equilibrium, the complete set of potential and kinetic energy parameters in a quadratic Euler–Langevin model can be explicitly characterized in terms of expected values of certain kinematic functions. The expected values could be approximated by averages over static data as would be obtained from X-ray diffraction studies of crystal structures or over dynamic data as would be obtained from atomistic-type molecular dynamics simulations. The characterizations derived here are properly consistent with the canonical measure on full phase space and involve a Jacobian factor, which causes the measure on configuration space to be non-Gaussian even though the potential energy is quadratic. While such factors are often ignored, or equivalently assumed to be constant, we include them here. Moreover, because they are entirely geometric and explicit functions of the internal coordinates, these factors can be included without additional effort in any scheme, numerical or experimental, to estimate material parameters. In applications to DNA, a challenging problem is to determine estimates for the potential energy and mass parameters in various different Euler–Langevin models as a function of the basepair sequence. Large data sets of molecular dynamics simulations have been prepared to this end [4, 10, 32]. Parameter extraction from the equilibrium distribution of an assumed stationary molecular dynamics times series has recently been performed using the theory outlined here; see [30] for details.

We stress that the structure and interpretation of our basic Euler–Langevin model were assumed from the outset. It is an interesting question whether such a model could be derived from first principles by considering a rigid body coupled to a heat bath

of water molecules. A derivation along these lines is likely to be formidable due in part to the need for defining an appropriate coupling between the body and bath. We have not attempted any such derivation here, but note that some results pertaining to the free, unforced motion of a convex body in an ideal gas heat bath can be found in [12]. Moreover, we remark that, although our model is of the multiplicative-noise type, there is no loss of generality in adopting an Itô interpretation. Indeed, due to the form of the coefficients in the model, the Itô and Stratonovich interpretations are equivalent. In the high-friction limit of the model, however, the two interpretations would in general be distinct.

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