Kinematic Basis of Emergent Energetic Descriptions of General Stochastic Dynamics

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We show a stochastic, kinematic description of a dynamics has a hidden energetic and thermodynamic structure. An energy function \( \varphi(x) \) emerges as the limit of the generalized free energy of the stochastic dynamics with vanishing noise. In terms of the \( \varphi \) and its orthogonal field \( \gamma(x) \perp \nabla \varphi \), a general vector field \( b(x) \) is decomposed into \( -D(x)\nabla \varphi + \gamma \), where \( \nabla : (\omega(x)\gamma(x)) = -\nabla \omega D(x)\nabla \varphi \), \( D(x) \) and \( \omega(x) \) represent the local geometry and density in the state space at \( x \). \( \varphi(x) \) and \( \omega(x) \) are interpreted as the emergent energy and degeneracy of the motion, with energy balance equation \( d\varphi(x(t))/dt = \gamma D^{-1} \gamma - bD^{-1} b \). The partition function and J. W. Gibbs’ method of statistical ensemble change naturally arise. The present theory provides a mathematical basis for P. W. Anderson’s emergent behavior in the hierarchical structure of science.

INTRODUCTION

Classical mechanics has traditionally been divided into kinematics and dynamics. The former gives the precise relationship between a mechanical motion \( x(t) \) described in terms of its velocity \( \dot{x}(t) \) or acceleration \( \ddot{x}(t) \) under geometric constraints, and the latter provides relationships between the motions and the concepts of mass, force, and mechanical energy. The former is a part of calculus, while the latter is based on Newton’s laws of motion. When a mechanical system contains a great many number of atoms and molecules, the notions of heat and temperature as a stochastic description of mechanical motion and kinetic energy, arises.

In classical, macroscopic chemical kinetics, a chemical reaction in aqueous solution, say \( A + B \rightarrow C \), is described by a rate process: \( d[A]/dt = -r(t) \), which should be identified as the chemical kinematics, while the functional relationship between \( r(t) \) and the \( c_A(t) \) and \( c_B(t) \), known as a rate law, can be identified as the chemical dynamics. One well-known example of a rate law is the mass action kinetics: \( r(t) = kc_A(t)c_B(t) \) where \( k \) is a constant independent of \( c_A \) and \( c_B \). It is clear that the former is again based on calculus which rigorously defines the concept of instantaneous rate of concentration change (fluxion), while the latter is a “natural law” with only an appropriate range of applicability. Chemical thermodynamics of homogeneous substances was developed by J. W. Gibbs, who introduced the notion of Gibbs function and chemical potential as the energy and force that drives the chemical changes.

With the above understandings, therefore, it came as a surprise that a recent work \([1,2]\) claims that the mathematical foundation of Gibbsian chemical thermodynamics needs only the mesososcopic stochastic kinematics, irrespective of any details of the rate laws. The implication of this observation is conceptually significant: It implies any stochastic, kinematic description of a complex dynamics has a hidden dynamical law that is defined by mathemaics! The present paper reports new results, obtained from exploring this idea, in the general stochastic dynamics in continuous state space \( x \in \mathbb{R}^n \) with continuous time \( t \in \mathbb{R} \). Mathematical analysis reveals the hidden thermodynamic structure that underlying the detailed kinematics. By “thermo”, we mean a stochastic description of a complex dynamics.

Our result is not as unorthodox as it seems: The concept of thermodynamic force was clearly articulated in the work of L. Onsager \([3]\). In chemical kinetics, it is widely accepted that entropic force is a legitimate force on par with mechanical force as a “cause” for an action. Entropy, however, is computable in any statistical description of dynamics \([4,5]\). Similarly, P. W. Anderson has stated that “[A]t each level of complexity entirely new properties appear, and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other.” \([6]\) In fact, he continued to provide a recipe for discovering an emergent law:

“It is only as the nucleus is considered to be a many-body system — in what is often called the \( N \rightarrow \infty \) limit — that such [emergent] behavior is rigorously definable. ... Starting with the fundamental laws and a computer, we would have to do two impossible things — solve a problem with infinitely many bodies [e.g., zero fluctuations], and then apply the result to a finite system — before we synthesized this behavior.”

As we shall see, the discovery of the hidden thermodynamic laws indeed involves taking the limit of noise tending zero. Our result also provides a clear understanding of why and how emergent thermodynamic behaviors, as statistical laws, can be independent of the details of the underlying dynamics.

We consider the general description of complex dynamics in terms of a stochastic process \( X_r(t) \). Such a dynamics can be characterized by its probability distribution \( p_r(x,t) \) that follows a Fokker-Planck equation \([7]\)

\[
\frac{\partial p_r}{\partial t} = -\nabla \cdot J[p_r], \quad J[p_r] \equiv b(x)p_r - \epsilon D(x)\nabla p_r, \quad (1)
\]

and its trajectory can be represented in terms of the solution to a Langevin type equation \( dX_r(t) = b(X_r)dt + [2\epsilon D(X_r)]^{1/2}dB(t) \), where \( B(t) \) is standard Brownian motion. The \( \epsilon \) is introduced to emphasize a connection between deterministic and stochastic motions \([8]\). In the limit of \( \epsilon \rightarrow 0 \), the stochastic trajectory \( X_r(t) \rightarrow \hat{x}(t) \) which satisfies \( d\hat{x}(t)/dt = b(\hat{x}(t)) \), and similarly \( p_r(x,t) \rightarrow \delta(x - \hat{x}(t)) \) if initial value \( p_r(x,0) = \delta(x - \hat{x}(0)) \).
In addition to the above straightforward limits, a mathematically-thermodynamic structure emerges in the process of taking the limit of $\epsilon \to 0$: For a fixed $\epsilon$ and regarding the general stochastic dynamics in (1), it is widely known that a free energy like quantity

$$\mathcal{F}[\pi_{\epsilon}(x,t)] = \int_{\mathbb{R}^n} p_{\epsilon}(x,t) \ln \left( \frac{p_{\epsilon}(x,t)}{\pi_{\epsilon}(x)} \right) dx,$$  \quad (2)

has a paramount importance [22-31], where the stationary solution to (1) $\pi_{\epsilon}(x)$ embodies the notion of an entropic force. More recently, it was discovered that the $\mathcal{F}$ actually satisfies a balance equation $d\mathcal{F}/dt = -f_{\epsilon}(t) - e_{\epsilon}(t)$ [12,15], with

$$f_{\epsilon}(t) = \int_{\mathbb{R}^n} J[\pi_{\epsilon}] \nabla \ln \left( \frac{p_{\epsilon}(x,t)}{\pi_{\epsilon}(x)} \right) dx,$$  \quad (3a)

$$Q_{hk}[\pi_{\epsilon}] = \int_{\mathbb{R}^n} J[\pi_{\epsilon}] (\epsilon D)^{-1}(x) J[\pi_{\epsilon}^{-1}(x)] dx,$$  \quad (3b)

$$e_{\epsilon}[\pi_{\epsilon}] = \int_{\mathbb{R}^n} J[\pi_{\epsilon}^{-1}(x)] J[\pi_{\epsilon}] p_{\epsilon}^{-1} dx.$$  \quad (3c)

All three quantities in (3) are non-negative. This fact ensures the interpretation of $Q_{hk}$ and $e_{\epsilon}$ as the source and sink for the free energy of a system. The $\mathcal{F}[\pi_{\epsilon}]$ is interpreted as a generalized free energy since $-\epsilon \int_{\mathbb{R}^n} p_{\epsilon} \ln \pi_{\epsilon} dx$, $\int_{\mathbb{R}^n} p_{\epsilon} \ln p_{\epsilon} dx$, and $\epsilon$ are analogous to “mean internal energy” $E$, entropy $S$, and temperature $T$, thus $\mathcal{F} = E - TS$. See [16-18] for the relation between these averaged thermodynamic quantities and the trajectory-based thermodynamics, Jarzynski equalities, and fluctuation theorems.

The new result of the present work is the complete system of three equations in Eq. (13), as an emergent description of the deterministic vector field $b(x)$. Among the three equations, the first two can be found in the mathematical work of Ventsel and Freidlin and the studies in physics that followed [19-21]. The (13a) is not the Helmholtz (or Hodge) decomposition of a vector field because $\gamma(x)$ is not divergence free (22). The motion following $\gamma(x)$ however, conserves the $\varphi(x)$ according to (13b). The divergence of $\gamma(x)$ is provided by the new equation (13c). The emergence of the $\omega(x)$ indicates the significance of a “local” invariant density of this $\varphi$-conservative motion [23]: This is called degeneracy in the classical statistical mechanical terminology. While the motion following $\gamma(x)$ can be complex, a statistical description, e.g., physical measure, usually exists [24,25]. For an extensive discussion of the thermodynamic meanings of dissipative vs. conservative motions, and their relation to trajectory-based entropy production, see [8,22].

**EMERGENT POTENTIAL $\varphi$ AND $\varphi$-CONSERVATIVE MOTION $\gamma$**

The mathematical theory of large deviations connects the stochastic dynamics with finite $\epsilon$ to the deterministic dynamics with $\epsilon = 0$ [26-31]. It is a rigorous and complete asymptotic theory akin to the WKB ansatz:

$$p_{\epsilon}(x,t) = \exp \left[ -\varphi_{\epsilon}^d(x,t)/\epsilon + o(\epsilon^{-1}) \right],$$  \quad (4)

in which $\varphi_{\epsilon}^d(x,t)$ is known as a time-dependent large deviation rate function. Taking the (4) as given and recall that $p_{\epsilon}(x,t) \to \delta(x-x(t))$, then it is easy to see that in the limit of $\epsilon \to 0$,

$$\epsilon \mathcal{F}[\pi_{\epsilon}(x,t)] \to \varphi^s(\hat{x}(t)), \quad \varphi^s(x) = -\lim_{\epsilon \to 0} \epsilon \ln \pi_{\epsilon}(x).$$  \quad (5)

Since $d\mathcal{F}/dt = -f_{\epsilon} \leq 0$, $\mathcal{F}[\pi_{\epsilon}(x,t)]$ is a monotonic non-increasing function of $t$. Consequently, (5) states that $\varphi^s(\hat{x}(t))$ is a monotonic function of $t$, which implies that $\varphi^s(x)$ is an energy function of the dissipative dynamics $\hat{x}(t)$, the solution to the deterministic equation $dx/dt = b(x)$. We shall drop the superscript from the steady-state large deviation rate function $\varphi^s(x)$ from now on.

The connection between $\mathcal{F}[\pi_{\epsilon}]$ and $\varphi(x)$ illustrates that the latter is an emergent energetic quantity in the limit of $\epsilon \to 0$. It provides a new proof with thermodynamic insights of the mathematical result of Ventsel and Freidlin [19-21]. The relation firmly connects (mesoscopic) stochastic free energy $\mathcal{F}[\pi_{\epsilon}]$ with (macroscopic) deterministic pseudo-potential $\varphi(x)$; it validates the earlier interpretation of $-\epsilon \int_{\mathbb{R}^n} p_{\epsilon} \ln \pi_{\epsilon} dx$ as a mean internal energy, with $\varphi(x)$ as the internal energy function of state $x \in \mathbb{R}^n$.

We emphasize that the original $b(x)$ in (1) is not a gradient field in general. In terms of the new found $\varphi(x)$ and continue the WKB ansatz, one can express

$$\pi_{\epsilon}(x) = \omega(x) \exp \left[ -\varphi(x)/\epsilon + a \ln \epsilon + O(\epsilon) \right],$$

in which $\ln \omega(x)$ is the next order to the leading two terms and $a \ln \epsilon$ arising from normalization factor is independent of $x$. Substituting this expression into

$$\nabla \left( \epsilon D(x) \nabla \pi_{\epsilon}(x) - b(x) \pi_{\epsilon}(x) \right) = 0,$$  \quad (6)

one obtains

$$\frac{\omega(x) \gamma(x) \cdot \nabla \varphi}{\epsilon} = \left[ \nabla \omega(x) \cdot D(x) \nabla \varphi + \nabla \cdot \left( \omega(x) \gamma(x) \right) \right] + \epsilon \nabla \cdot \left( D(x) \nabla \omega(x) \right) + O(\epsilon) = 0,$$  \quad (7)

in which $\gamma(x) = D(x) \nabla \varphi(x) + b(x)$. Equating like order terms in (7), we have

$$\nabla \varphi(x) \cdot \gamma(x) = 0, \quad \forall x \in \mathbb{R}^n,$$  \quad (8)

the vector field $\gamma(x)$ is orthogonal to $\nabla \varphi(x)$, and

$$\nabla \cdot \left( \omega(x) \gamma(x) \right) = -\nabla \omega(x) \cdot D(x) \nabla \varphi(x).$$  \quad (9)

Actually for finite $\epsilon$,

$$\Pi_{\epsilon}(x) = \pi_{\epsilon}^{-1}(x) J \left[ \pi_{\epsilon}(x) \right] = b(x) - cD(x) \nabla \ln \pi_{\epsilon}(x),$$  \quad (10)
Stochastic systems with $\epsilon$ in which the vector fields are driven\cite{37,38}, which is expected to approach to an equilibrium $\Pi$ onsager's thermodynamics force, $\Pi = \epsilon \nabla \cdot \epsilon \Pi$. Therefore, taking the limit $\epsilon \to 0$ we have

$$\lim_{\epsilon \to 0} \Pi_{\epsilon}(x) = b(x) + D(x)\nabla \phi(x) \equiv \gamma(x). \quad (11)$$

The vector fields following the vector field $\gamma(x)$ is restricted on the level set of $\phi(x)$. To see the orthogonality, let us denote $\phi_{\epsilon}(x) = -\epsilon \ln \pi_{\epsilon}(x)$, which has been widely called a kinetic potential\cite{33,35}. Then the stationary Fokker-Planck equation \ref{31} in fact can be re-written as an inner-product formula that is valid for all $\epsilon > 0$\cite{33,36}:

$$\nabla \phi_{\epsilon}(x) \cdot \Pi_{\epsilon}(x) = \epsilon \nabla \cdot \Pi_{\epsilon}(x). \quad (12)$$

Therefore, if $\nabla \cdot \Pi_{\epsilon} = 0$, then there is an orthogonality between $\nabla \phi_{\epsilon}(x)$ and $\Pi_{\epsilon}(x)$ for finite $\epsilon$. On the other hand, in the limit of $\epsilon \to 0$, $\phi_{\epsilon}(x) \to \phi(x)$, $\Pi_{\epsilon} \to \gamma$, and $\gamma \cdot \nabla \phi = 0$.

$\gamma(x) = 0$ is mathematically equivalent to detailed balance. Stochastic systems with $\gamma = 0$ is widely considered as “non-driven”\cite{37,38}, which is expected to approach to an equilibrium steady state in the long-time limit. For such systems, the free energy $F$ acquires additional meaning as the potential of Onsager’s thermodynamics force, $\Pi_{\epsilon} = D(x)\nabla F$.

Collecting Eqs. \ref{11} and \ref{8}, we have a system of three equations

$$b(x) = -D(x)\nabla \phi(x) + \gamma(x), \quad (13a)$$

$$\nabla \phi(x) \cdot \gamma(x) = 0, \quad (13b)$$

$$\nabla \cdot (\omega(x)\gamma(x)) = -\nabla \omega(x) \cdot D(x)\nabla \phi(x), \quad (13c)$$

in which the vector fields $b(x)$ and $\gamma(x)$ represent dynamics, $D(x)$, which represents stochastic motion, can be thought as a geometric metrics, $\omega(x)$ represents local “measure” (degeneracy in the classical statistical mechanical terminology), and $\phi(x)$ and $\ln \omega(x)$ are thermodynamic quantities akin to energy and entropy, respectively. The “noise structure” $D(x)$ provides a unique geometry for the dynamics. In the simplest case, if $D(x)$ is the identity matrix, and $\omega(x) = 1$ is the Lebesgue measure, then the equations in \ref{13} become

$$b(x) = -\nabla \phi(x) + \gamma(x), \quad (14a)$$

$$\gamma(x) \cdot \nabla \phi(x) = 0, \quad (14b)$$

$$\nabla \cdot \gamma(x) = 0. \quad (14c)$$

The vector field $\gamma(x)$ is now volume preserving and it also has a conserved quantity $\phi(x)$. System in \ref{14} is intimately related to the classical Hamiltonian systems\cite{39}. One of the most important features of this class of dynamics is that the $\phi(x)$ gives the steady state probability distribution exactly for any finite $\epsilon$ in the form of $\pi_{\epsilon}(x) \propto e^{-\phi(x)/\epsilon}$ according to Boltzmann’s law, if one identifies $\epsilon$ with temperature \cite{8,22}.

\[ \varphi\text{-BASED STATISTICAL MECHANICS AND ENSEMBLE CHANGE} \]

It is seen immediately that if one computes a partition function from energy function $\phi(x)$ and degeneracy $\omega(x)$:

$$Z(\epsilon) = \int_{\mathbb{R}^n} \omega(x)e^{-\phi(x)/\epsilon} dx, \quad (15)$$

then $Z^{-1}(\epsilon)\omega(x)e^{-\phi(x)/\epsilon}$ is the asymptotic probability density for $\pi_{\epsilon}(x)$. If the principle of equal probability is valid, e.g., $\nabla \cdot \gamma(x) = 0$, then it is the stationary probability density of $\Pi$ for all $\epsilon > 0$.

Let us now consider a bivariate stochastic dynamics with $x$ and $y$ which is assumed to be a scalar for simplicity. The stationary joint probability for $x$ and $y$, $p_{\epsilon}(x,y)$ is related to the stationary conditional probability $p_{\epsilon}(x|y)$ through the marginal distribution for variable $y$, $p_{\epsilon,y}(y): p_{\epsilon}(x,y) = p_{\epsilon}(x|y)p_{\epsilon,y}(y)$. In the asymptotic limit of $\epsilon \to 0$, this yields

$$\phi(x,y) = \phi(x|y) + \phi_y(y), \quad (16)$$

and the partition functions

$$Z_{x,y}(\epsilon) = \int_y Z_{x|y}(\epsilon;y)e^{-\phi_y(y)/\epsilon} dy. \quad (17)$$

The $Z_{x|y}$ is the partition function with fixed $y$, treated as a parameter, and $Z_{x,y}$ is the partition function with fluctuating $y$. To asymptotically evaluating the integral in \ref{17}, it can be shown that at $y = \overline{y}$, the mean value of the fluctuating $y$:

$$\frac{\partial}{\partial y} \phi_y(\overline{y}) = \epsilon \left[ \frac{\partial}{\partial y} \ln Z_{x|y}(\epsilon;y) \right]_{y=\overline{y}} \equiv \xi_y, \quad (18)$$

where $\xi_y$ is the conjugate variable to $y$. Therefore, the integrand in \ref{17} can be approximately expressed as

$$\phi_y(y) \simeq \phi_y(\overline{y}) + \xi_y(y - \overline{y}). \quad (19)$$

Eqs. \ref{17} and \ref{18} constitute J. W. Gibbs’ theory of ensemble change. In doing so, the thermodynamics of a stationary system with fluctuating $y$ and the thermodynamics of a stationary system with fixed $y$ are logically connected via the large deviation theory. This derivation shares the same spirit as Helmholtz and Boltzmann’s 1884 mechanical theory of heat\cite{40,41}. Both extend the notion of energy from a system with a fixed “parameter” $y$ to an entire family of systems with different $y$’s\cite{42}.

\[ \text{AN INSTANTANEOUS DETERMINISTIC ENERGY BALANCE EQUATION} \]

While the $\epsilon F[p_{\epsilon}(x,t)] \to \phi(x(t))$ as $\epsilon \to 0$ and $p_{\epsilon}(x,t) \to \delta(x - \overline{x}(t))$, the free energy dissipation, housekeeping heat, and entropy production rates\cite{12,15}, also
known as non-adiabatic, adiabatic, and total entropy production rates \([14]\), become
\[
e_{f_d}[p_u(x, t)] \rightarrow \left[ \nabla \varphi(x) \mathbf{D}(x) \nabla \varphi(x) \right]_{x=x(t)} , \tag{20a}
\]
\[
e_Q[h_k][p_v(x, t)] \rightarrow \left[ \gamma(x) \mathbf{D}^{-1}(x) \gamma(x) \right]_{x=x(t)} , \tag{20b}
\]
\[
e_{e_p}[p_r(x, t)] \rightarrow \left[ \mathbf{b}(x) \mathbf{D}^{-1}(x) \mathbf{b}(x) \right]_{x=x(t)} . \tag{20c}
\]

All three quantities are non-negative. They are linked through a Pythagorean-like equation, \(\forall x \in \mathbb{R}^n:\)
\[
\| \mathbf{D}(x) \nabla \varphi(x) \|^2 + \| \gamma(x) \|^2 = \| \mathbf{b}(x) \|^2 , \tag{21}
\]
under the inner product \((u, v) \equiv v \cdot \mathbf{D}^{-1} u\) and thus \(\| u \|^2 = u \mathbf{D}^{-1} u.[2]\)

In the zero-noise limit, the deterministic motion follows \(dx(t)/dt = \mathbf{b}(x)\); the balance equation \(dF/dt \equiv -f_d = Q_{h_k} - e_p\) now becomes
\[
\frac{d}{dt} \varphi(x(t)) = \mathbf{b}(x) \cdot \nabla \varphi(x)
= \gamma(x) \mathbf{D}^{-1}(x) \gamma(x) - \mathbf{b}(x) \mathbf{D}^{-1}(x) \mathbf{b}(x) . \tag{22}
\]

Both terms before and after the minus sign in (22) are non-negative. Eq. (22) constitutes a deterministic, instantaneous energy balance law with the non-conservative pump as the source and energy dissipation as the sink, respectively. This result provides a rigorous notion of “energy” for complex dynamics with a stochastic kinematic description. For a classical mechanical system with potential force and friction, \(\varphi\) is the sum of kinetic energy and potential energy, and the energy dissipation is due to the friction.

**DISCUSSION**

In the theory of ordinary differential equations, Hamiltonian dynamics with the conserved \(H\) function and gradient systems with energy functions are two special cases that have been extensively studied \([29]\). For a general nonlinear dynamics \(x = \mathbf{b}(x)\), it is not known whether it always has an associated “energetics”. Ventsel and Freidlin’s large deviation theory revealed that with the presence of a noise, a global quasi-potential function \(\varphi(x)\) exists \([12, 21]\). The present work further shows that the deterministic vector field \(\mathbf{b}(x) = \mathbf{D}(x) \nabla \varphi(x) + \gamma(x)\), where \(\gamma(x) \perp \nabla \varphi(x)\) at every \(x\), also has \(\nabla \cdot (\omega(x) \gamma(x)) = -\nabla \omega(x) \cdot \mathbf{D}(x) \nabla \varphi(x)\). This is a general result of which the conservative dynamics and gradient systems are special cases.

If one calls \(\mathbf{x} = \mathbf{b}(x)\) kinematic description of a complex dynamics, then the system \([13]\) and Eq. (22) provide an energetic description that is hidden under the kinematics. A few words concerning the role of \(\mathbf{D}(x)\) are in order. The concept of a gradient field on \(\mathbb{R}^n\) requires a notion of \textit{distance}. This is naturally provided by the noise structure embedded in \(\mathbf{D}(x)\).

This is precisely A. N. Kolmogorov’s insights on the nature of probability theory: One needs to have a \textit{a priori} before carrying out a probabilistic computation.

For complex systems, not all “stochasticity” are due to thermal noises. In fact, the Mori-Zwanzig theory of projection operator clearly shows that \([43]\) the dynamics of a projection necessarily has, in general, a stochastic term and a non-Markovian memory term.

When \(\gamma = 0\), the Fokker-Planck equation in \([11]\) is a gradient flow in a proper mathematical space \([49]\). In terms of the Pythagorean-like equation in \([21]\), the stochastic dynamics following the \([11]\) with \(\gamma = 0\) has a maximal \(f_d\). One leg has the same length as the triangle’s hypotenuse. Thus, under an appropriate geometry, Onsager’s principle of maximum dissipation can be generalized to nonlinear regime \([44]\). In recent years, the theory of nonequilibrium landscape has gained wider recognitions in biological physics \([45, 47, 48]\). Since for a nonequilibrium stochastic system, its stationary state still has highly complex motions as NESS flux \([37, 38, 47]\), the \(\varphi\) is only half the story: the \(\gamma\) and its related \(\omega\) provide the characterization of the NESS motion on each and every \(\varphi\) level set.

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