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Supplemental Material: Coupled Nosé-Hoover Equations of Motions

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Abstract

Details of mathematical aspects and trajectories of control variables are described for a text entitled “Coupled Nosé-Hoover Equations of Motions.”

Note: An equation such as "Eq. (1)" refers to the equation that appears in the text, while an equation such as "Eq. (S1)" refers to the equation that appears in this document.

I. EVALUATION OF ϵ

The value of $\epsilon_i(\beta_0) \in \mathbb{R}$ ($i = 1, \dots, m$), defined by Eq. (45), can be evaluated, under suitable mathematical conditions, such that

$$\epsilon_i(\beta_0) = - \int_{\mathbb{R}^{2n}} D_{\beta_i} \rho_E(E(x, p), \beta_0) dx dp \Bigg/ \int_{\mathbb{R}^{2n}} \rho_E(E(x, p), \beta_0) dx dp \quad (\text{S1a})$$

$$= - \int_{\mathbb{R}^{2n}} \rho_E(E(x, p), \beta_0) D_{\beta_i} \ln \rho_E(E(x, p), \beta_0) dx dp \Bigg/ \int_{\mathbb{R}^{2n}} \rho_E(E(x, p), \beta_0) dx dp \quad (\text{S1b})$$

$$= \left\langle Y_i^{\beta_0} \right\rangle_{\rho_E; \beta_0}, \quad (\text{S1c})$$

where $Y_i^{\beta_0}(x, p) \equiv -D_{\beta_i} \ln \rho_E(E(x, p), \beta_0)$ for $(x, p) \in \mathbb{R}^{2n}$. Namely, $\epsilon_i(\beta_0)$ is the average of the function $Y_i^{\beta_0}$ in the distribution whose density, $\rho_0(x, p, \dots)$, is proportional to $\rho_E(E(x, p), \beta_0)$. Note that β_0 is not a dynamical variable here, but just an arbitrarily fixed parameter value. By using e.g., the density dynamics [Phys. Rev. E **65**, 026105 (2002); *ibid.* **71**, 046708 (2005)], such a density ρ_0 can be created, so that $\epsilon_i(\beta_0)$ is obtained as the long-time average, generated by the density dynamics, of $Y_i^{\beta_0}$ in principle. Note that if $m = 1$ and ρ_E is the BG density, then $\epsilon(\beta_0)$ is the energy average under the BG ensemble at temperature $1/k_B\beta_0$.

II. THE SOLUTION OF THE INVERSE PROBLEM

Consider s approximate equalities,

$$\langle h_\nu(\beta) \rangle \simeq \gamma_\nu \in \mathbb{R}, \quad \nu = 1, \dots, s, \quad (\text{S2})$$

for given values, $(\gamma_1, \dots, \gamma_s) = \gamma$, in general [$s = 1$ is used in Eq. (65)]. Here the LHS is defined using a given function f that contains l ($\geq s$) parameters $(\alpha_1, \dots, \alpha_l) = \alpha \in \mathbb{R}^l$; viz., $f = f(\cdot; \alpha) : \sigma(\mathbb{R}^m) \rightarrow \mathbb{R}$, $\beta \mapsto f(\beta; \alpha)$. We solve Eq. (S2) with respect to α for a given γ . To do this, we assume three conditions: (i) for any given $\beta_0 \in \sigma(\mathbb{R}^m)$, there exists $U_0 \equiv \mathcal{E}(\beta_0) \in \mathbb{R}^M$ ($M \in \mathbb{N}$) such that

$$\epsilon(\beta_0; U_0) \simeq 0, \quad (\text{S3})$$

where $\epsilon(\beta_0; U_0)$ is defined in Eq. (47); (ii) we can represent such that $\beta_0 = \lambda(\alpha)$, where the mapping $\lambda : \mathbb{R}^l \rightarrow \sigma(\mathbb{R}^m)$ is specifically computed; (iii) for a map $\Phi = (\Phi_1 \dots, \Phi_s)$ defined by $\Phi_\nu(\alpha) \equiv \langle h_\nu \rangle_{f(\cdot; \alpha)}$ ($\nu = 1, \dots, s$), there exists $\alpha \in \mathbb{R}^l$ such that

$$\Phi(\alpha) = \gamma \quad (\text{S4})$$

for a given $\gamma \in \mathbb{R}^s$.

Now, take a solution (which is not necessarily unique) of Eq. (S4), $\alpha_\gamma \in \mathbb{R}^l$ [assumption (iii)]. Then we have $\beta_0 = \beta_0^\gamma \equiv \lambda(\alpha_\gamma)$ [assumption (ii)], and set $U_0 = U_0^\gamma \equiv \mathcal{E}(\beta_0^\gamma)$ that yields $\epsilon(\beta_0^\gamma; U_0^\gamma) \simeq 0$ [assumption (i)]. Remember that we have α_γ , β_0^γ , and U_0^γ for the given γ in advance. We thereby see that α_γ also becomes a solution of Eq. (S2), because

$$\left. \frac{\int_{\sigma(\mathbb{R}^m)} h_\nu(\beta) f(\beta; \alpha) Z(\beta; U_0) d\beta}{\int_{\sigma(\mathbb{R}^m)} f(\beta; \alpha) Z(\beta; U_0) d\beta} \right|_{\substack{\alpha=\alpha_\gamma, \\ U_0=U_0^\gamma}} \equiv \langle h_\nu(\beta) \rangle \Big|_{\substack{\alpha=\alpha_\gamma, \\ U_0=U_0^\gamma}} \quad (\text{S5a})$$

$$\simeq \left. \frac{\int_{\sigma(\mathbb{R}^m)} h_\nu(\beta) f(\beta; \alpha) e^{-(\epsilon(\beta_0; U_0)|\beta)} d\beta}{\int_{\sigma(\mathbb{R}^m)} f(\beta; \alpha) e^{-(\epsilon(\beta_0; U_0)|\beta)} d\beta} \right|_{\substack{\alpha=\alpha_\gamma, \beta_0=\beta_0^\gamma, \\ U_0=U_0^\gamma=\mathcal{E}(\beta_0^\gamma)}} \equiv \langle \langle h_\nu(\beta) \rangle \rangle \Big|_{\substack{\alpha=\alpha_\gamma, \beta_0=\beta_0^\gamma, \\ U_0=U_0^\gamma}} \quad (\text{S5b})$$

$$\simeq \left. \frac{\int_{\sigma(\mathbb{R}^m)} h_\nu(\beta) f(\beta; \alpha) d\beta}{\int_{\sigma(\mathbb{R}^m)} f(\beta; \alpha) d\beta} \right|_{\alpha=\alpha_\gamma} \equiv \langle h_\nu \rangle_{f(\cdot; \alpha_\gamma)} \quad (\text{S5c})$$

$$= \Phi_\nu(\alpha_\gamma) = \gamma_\nu \quad (\text{S5d})$$

holds for any ν .

Note that, while assumptions (ii) and (iii) may be loosened for small l , m , and s , assumption (i) should be critical to solve the problem. To specifically see this, suppose an ideal situation where the integration, Eq. (46b), is explicitly performed so that $\langle \langle h(\beta) \rangle \rangle$ is given by a known function, Ψ , of both $\epsilon(\beta_0)$ and α ; viz., $\langle \langle h(\beta) \rangle \rangle = \Psi(\epsilon(\lambda(\alpha)), \alpha)$. Nonetheless, we cannot easily solve $\Psi(\epsilon(\lambda(\alpha)), \alpha) = \gamma$ with respect to α , since the function ϵ is unknown [much effort is required to know the entire functional form; cf. Eq. (S1)], although the functions Ψ and λ are known (by the assumptions).

III. THE EFFECT OF PARAMETER c

A special case.—We investigate the effect of parameter c introduced in Eq. (55). First we consider the function setting in Sec. II I in the text, where ρ_E is given by Eq. (53), or its generalization, Eq. (59), and $f \equiv f_G$ is given by Eq. (56). Then the ODE is given

by Eq. (5) with $T(x, p, Q)$ represented by Eq. (54) and $\tilde{U}_\epsilon(Q)$ represented by Eq. (58) with $A_\epsilon = c(\epsilon + \alpha_2 + U_0)$. Let $\varphi : t \mapsto (x(t), p(t), \zeta(t), Q(t), \mathcal{P}(t), \eta(t))$ be any solution of ODE (5), $\dot{\omega} = X'(\omega)$. Suppose that we change the parameter value from $c > 0$ to $c' > 0$. We then have a number γ that satisfies $c' = e^{-\gamma/l}c =: c_\gamma$. Define a phase-space map $\nu_\gamma : \Omega \rightarrow \Omega, (x, p, \zeta, Q, \mathcal{P}, \eta) \mapsto (x, p, \zeta, Q + \gamma, \mathcal{P}, \eta)$, viz., the translation of Q . Then $\varphi_\gamma := \nu_\gamma \circ \varphi : t \mapsto (x(t), p(t), \zeta(t), Q(t) + \gamma, \mathcal{P}(t), \eta(t))$ is a solution of an ODE, $\dot{\omega} = X'_\gamma(\omega)$, where X'_γ is X' using c_γ instead of c . This is shown as follows: *For any ω , $X'_\gamma(\nu_\gamma(\omega)) = X'_\gamma(x, p, \zeta, Q + \gamma, P, \eta)$ is given by Eq. (10) [RHS of Eq. (5)] with $T_\gamma(x, p, Q + \gamma)$ and $\nabla \tilde{U}_{E(x,p)}^\gamma(Q + \gamma)$, instead of $T(x, p, Q)$ and $\nabla \tilde{U}_{E(x,p)}(Q)$, respectively. Here the index γ in T_γ and $\nabla \tilde{U}_{E(x,p)}^\gamma$ indicate the use of c_γ instead of c . We find that $T_\gamma(x, p, Q + \gamma) = 1/(k_B c_\gamma) e^{-(Q+\gamma)/l} = T(x, p, Q)$ and $\nabla \tilde{U}_{E(x,p)}^\gamma(Q + \gamma) = (c_\gamma/l)(E(x, p) + \alpha_2 + U_0) e^{(Q+\gamma)/l} - (\alpha_1 + 1)/l = \nabla \tilde{U}_{E(x,p)}(Q)$. Thus*

$$X'_\gamma(\nu_\gamma(\omega)) = X'(\omega) \text{ for all } \omega. \quad (\text{S6})$$

Therefore we have $D\varphi_\gamma(t) = D\nu_\gamma(\varphi(t)) \circ D\varphi(t) = D\varphi(t) = X'(\varphi(t)) = X'_\gamma(\nu_\gamma(\varphi(t))) = X'_\gamma(\varphi_\gamma(t))$ for all t , so the proof is completed.

Namely, the translation of Q in any solution of the original ODE just yields a solution of the parameter-changed ($c \rightarrow c_\gamma$) ODE. Conversely, for any solution, φ_γ , of $\dot{\omega} = X'_\gamma(\omega)$, we similarly see that $\nu_{-\gamma} \circ \varphi_\gamma$ becomes a solution of $\dot{\omega} = X'(\omega)$. Thus, we have a mapping between the solution spaces, $\mathcal{S} := \{\text{solution of } \dot{\omega} = X'(\omega)\} \rightarrow \mathcal{S}_\gamma = \{\text{solution of } \dot{\omega} = X'_\gamma(\omega)\}$, $\varphi \xrightarrow{d} \nu_\gamma \circ \varphi$, and find it is bijective, due to $\nu_\gamma \circ \nu_{-\gamma} = \text{id}_\Omega$ ($\forall \gamma$). This means that we completely know the solutions of the parameter-changed ODE from the solutions of the original ODE, just by the translation.

A general case.—The above results also hold in a more general function setting. Let the map $\sigma : \mathbb{R}^m \rightarrow \mathbb{R}^m$ be parameterized by $c \in A$ (a certain set), denoted as σ_c . We only assume two conditions. First, σ possesses the following relationship between a parameter change and a variable translation: for $c_1, c_2 \in A$, there exists $\gamma \in \mathbb{R}^m$ such that $\sigma_{c_2}(Q) = \sigma_{c_1}(Q - \gamma)$ for all Q (this σ_c is a generalization of the map $Q \mapsto ce^{Q/l}$ with $m = 1$). Second, the vector field, X_c , is smooth and takes the form: $X_c(\omega) = Y(x, p, \zeta, \mathcal{P}, \eta, \sigma_c(Q), D\sigma_c(Q), D^2\sigma_c(Q))$; viz., the dependence on Q is only through σ_c and its first and second differentials, $D\sigma_c$ and $D^2\sigma_c$ [Eq. (5) satisfies this condition, since $T(x, p, Q)$ given by Eq. (6) involves only $\sigma(Q)$ and since $\tilde{U}_{E(x,p)}$ given by Eq. (8) involves only $\sigma(Q)$ and $D\sigma(Q)$ [see also Eq. (3)] so that $\nabla \tilde{U}_{E(x,p)}(Q)$ involves only $D^k\sigma_c(Q)$ ($k = 0, 1, 2$)]. We can show that if φ is a solution of

$\dot{\omega} = X_{c_1}(\omega)$ then $\nu_\gamma \circ \varphi$ (ν_γ is the one given above) becomes a solution of $\dot{\omega} = X_{c_2}(\omega)$: It follows from $D^k \sigma_{c_2}(Q) = D^k \sigma_{c_1}(Q - \gamma)$ for every Q and k that $X_{c_2}(\nu_\gamma(\omega)) = X_{c_1}(\omega)$ for all ω , which corresponds to Eq. (S6). Hence the proof can be completed in the same manner as the special case. Similarly, a bijective mapping between the solution space of $\dot{\omega} = X_{c_1}(\omega)$ and that of $\dot{\omega} = X_{c_2}(\omega)$ is obtained.

IV. THE TOTAL ERROR

Figure 1 shows the total error measured by $\Delta(t)$, with respect to time t , for the distribution of x in the 1-dimensional double-well (1DW) potential system. See text for the details.

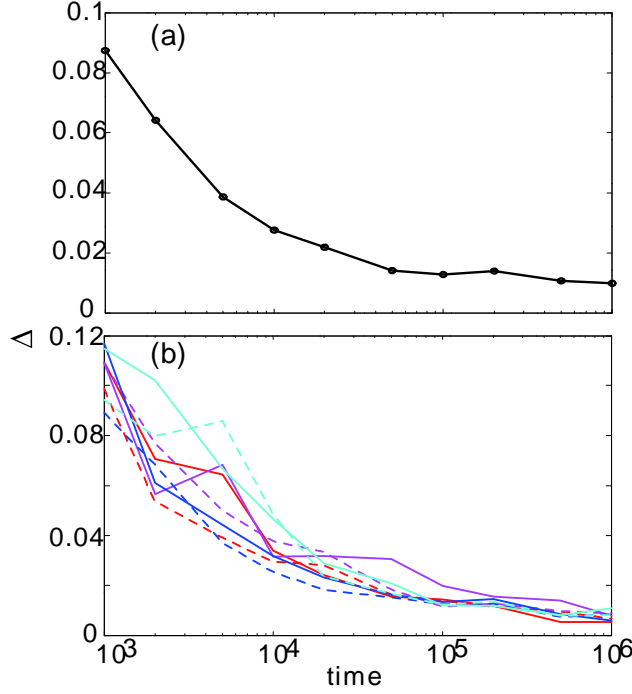


FIG. 1: (a) Difference in the 1D marginal distribution of x between simulation and theory as a function of the simulation time for the 1DW model. (b) The same as (a), but $c_Z = 0.1$ (solid, blue) and 10 (dashed, blue), $c_Y = 0.1$ (solid, cyan) and 10 (dashed, cyan), $\mathbf{M}_T = 0.1$ (solid, red) and 10 (dashed, red), and $l = 0.224$ (solid, magenta) and 22.4 (dashed, magenta). $c_Z = c_Y = 1$, $\mathbf{M}_T = 1$, and $l = 2.24$ are used unless otherwise mentioned. All quantities are dimensionless.

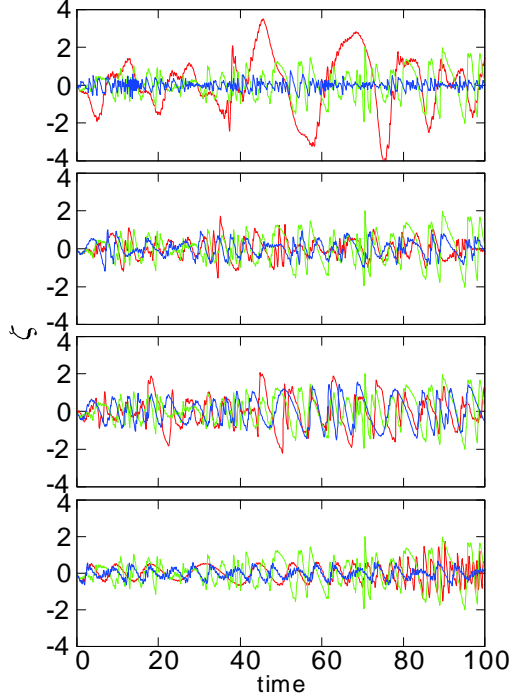


FIG. 2: Time courses of ζ for 1DW. Color schemes are the same as in Fig. 4 of the text.

V. TRAJECTORIES OF ζ , η , AND \mathcal{P} FOR THE 1DW MODEL SYSTEM

The oscillation, as well as the distribution, of ζ depends on c_Z , where a smaller c_Z tends to yield a larger period (Fig. 2). This is reasonable as an analogue that we observe in the single NH equation, because c_Z essentially corresponds to the inverse of Nose's mass Q_{NH} [recall the discussion in Sec. IIB in the text, such that the setting of our $\rho_Z(\zeta)$ leads to the friction term of the NH equation via $c_Z = 1/2k_B T_{\text{ex}} Q_{\text{NH}}$]. In contrast, ζ , which directly controls the physical system, depends minimally on c_Y and \mathbf{M}_T , as these are temperature-system parameters. The effects of l on the dynamics of ζ are not straightforward. ζ is governed by $\dot{\zeta} = T_P - T_D$ ($nk_B = 1$ in 1DW), as seen in the typical examples shown in Fig. 3. When $l = 22.4$ [Fig. 3(a)], around T_D , which reduces slowly, T_P oscillates fast, so that ζ has two oscillation modes: one is the slow (~ 3 periods for time 20) mode around zero with relatively large amplitudes and the other is the fast mode, inherited from T_P , with relatively small amplitudes. While for $l = 0.224$ [Fig. 3(b)], T_D and T_P oscillate with larger amplitudes than those in Fig. 3(a). However, since the periods of T_D and T_P are similar, cancellations occur so that $T_P - T_D$ maintains small values and the amplitude of ζ is comparable to that in

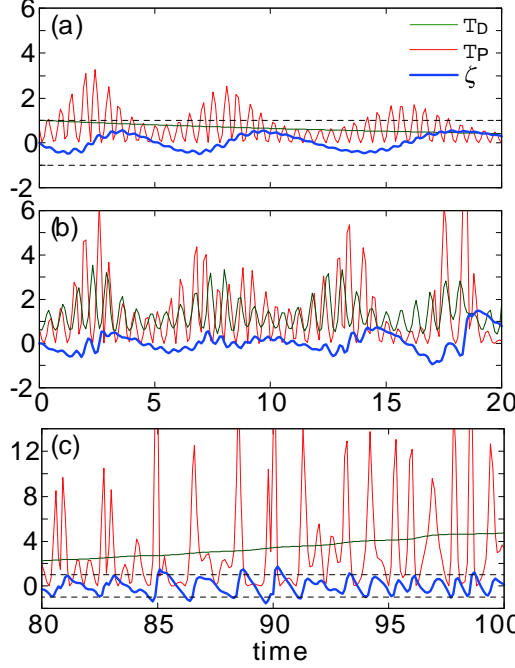


FIG. 3: Time courses of T_D (green) and T_P (red), and ζ (blue) for 1DW. (a) $l = 22.4$, $0 \leq t \leq 20$; (b) $l = 0.224$, $0 \leq t \leq 20$; and (c) $l = 22.4$, $80 \leq t \leq 100$. Dotted lines in (a) and (c) indicate ± 1 .

Fig. 3(a). For $l = 22.4$ and $80 \leq t \leq 100$ [Fig. 3(c)], against the slow motion of T_D as in $0 \leq t \leq 20$ [Fig. 3(a)], T_P oscillates with very large amplitudes [cf. Fig. 4(b) of the text], which affect the motion of ζ . The faster mode of ζ seen in $0 \leq t \leq 20$ seems to grow and attain the large amplitudes in $80 \leq t \leq 100$. This is the reason why ζ for $l = 22.4$ suddenly has the large fluctuations seen in Fig. 2 (bottom panel).

The trajectories of η show that a larger period and amplitude in the oscillating-like motion of η appear as c_Y is decreased (Fig. 4). This dependence of c_Y on η is similar to the dependence of c_Z on ζ , as expected from the roles of these two parameters [exactly speaking, there is a difference in that the friction term $\tau_Z(\zeta)$ described by ζ and c_Z in Eq. (5) is multiplied by $T(x, p, Q)$, whereas the friction term $\tau_Y(\eta)$ described by η and c_Y is not]. The temperature-system variable η does not strongly depend on the physical-system parameter c_Z . We also see that η —a control variable in the temperature system—does not strongly depend on the temperature-system parameters, \mathbf{M}_T , which is the mass parameter, and l , which is the potential parameter [see Eq. (58)]. This tendency seems to be reasonable, by considering the analogous tendency in the single NH equation that the control variable in

the physical system does not depend strongly on the mass and potential parameters of the physical system.

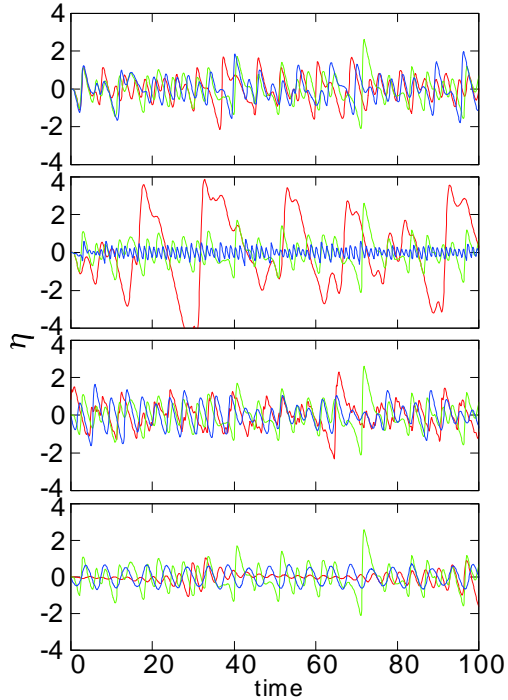


FIG. 4: Time courses of η for 1DW. Color schemes are the same as in Fig. 4 of the text.

The dependence on the parameters of the trajectory of \mathcal{P} (Fig. 5) is similar to that of the dynamical temperature T_D . This is suggested by the relations, $\mathbf{M}_T^{-1}\mathcal{P} = \dot{Q}$ and $T_D \propto \exp[-Q/l]$. Even though the cases of $c_Y = 10$ and $\mathbf{M}_T = 10$ are seemingly exceptional, the periods of the two oscillating modes existing in T_D and in \mathcal{P} are actually similar, whereas the faster modes in \mathcal{P} have large amplitudes and those in T_D have small amplitudes. As expected from the relation, $\dot{\eta} = \mathbf{M}_T^{-1}\mathcal{P}^2 - 1$, there are also correlations between \mathcal{P}^2 and η . This may not be clear for $l = 0.224$ in the behavior of \mathcal{P} shown in Fig. 5, but it is actually observed if we view them on a shorter time scale, as shown in Fig. 6.

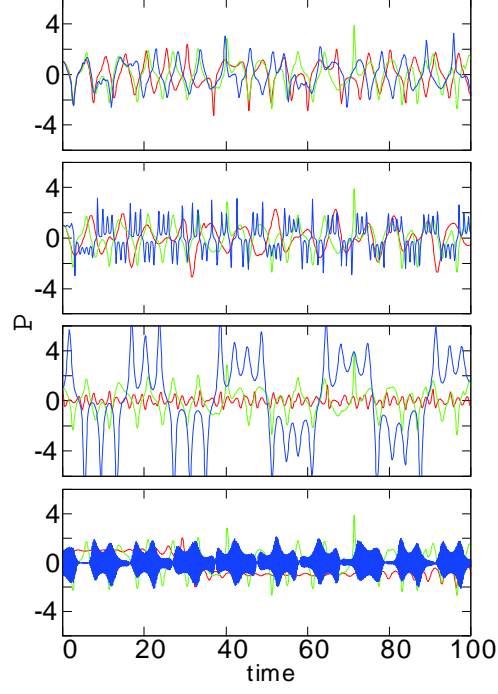


FIG. 5: Time courses of \mathcal{P} for 1DW. Color schemes are the same as in Fig. 4 of the text.

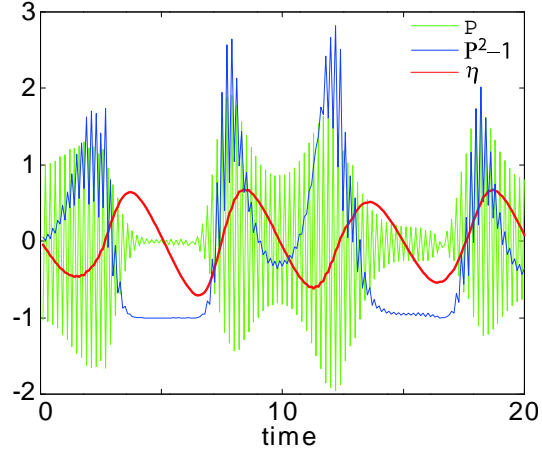


FIG. 6: Time courses of \mathcal{P} (green), $\mathcal{P}^2 - 1$ (blue) and η (red) for 1DW. $l = 0.224$ and $\mathbf{M}_T = 1$.