Enforced Swift Equilibrium on Manifolds

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ABSTRACT TO BE WRITTEN ,,,

I. INTRODUCTION

The story is a familiar one. We have a physical system with microstates X, each of which with potential $V(x;\lambda)$, whereby the λ's are control parameters we can manipulate. The probability distribution of the microstates then follows the Boltzmann Distribution:

$$\rho_{\text{eq}}(x;\lambda) = \big(Z(\lambda)\big)^{-1} \exp(-\beta V(x;\lambda)) \tag{1}$$

whereby $\beta = (k_B T)^{-1}$ is the inverse temperature (and perhaps yet another control parameter), and Z is the Boltzmann factor. In general, if you change $\lambda(t)$ slowly enough, the probability distribution $\rho(x, \lambda(t))$ remains infinitesimally close to $\rho_{\text{eq}}(x, \lambda(t))$ as specified by Equation 1. When you change $\lambda(t)$ faster than the relaxation timescale τ_{relax} (system-dependent), this is not the case. The million dollar question: is it possible to apply an external driving force to your system to offset the non-equilibrium perturbation terms, caused by changing $\lambda(t)$ in a non-adiabatic manner?

This is the problem of Enforced Swift Equilibrium that we are to solve and generalize to arbitrary Riemannian manifolds.

II. LANGEVIN DYNAMICS

In particular, we will start with consider a particle undergoing Browning motion in the overdamped regime, whose dynamics are governed by the Langevin equation:

$$\gamma \frac{d\vec{x}}{dt} = -\vec{\nabla} V(\vec{x};\lambda) + \vec{\eta}(t) + \vec{F}_{\text{ext}}(t) \tag{2}$$

whereby $\vec{x}$ is the position of the particle, γ is the viscosity, V_λ is the potential acting upon the particle, η is noise with autoc-orrelation $< \eta(t')\eta(t) >= (2\gamma/\beta)\delta(t'-t)$, and $\vec{F}_{\text{ext}}(t)$ is the external force we act upon the particle.

Supposing for now that both λ and $\vec{F}_{\text{ext}}$ are constants in time, the well-known solution of the Fokker-Planck equation would solve:

$$\partial_t \rho = \vec{\nabla} \cdot \left[\left(\frac{\vec{\nabla} V(\vec{x};\lambda) - \vec{F}_{\text{ext}}}{\gamma} + \frac{\vec{\nabla}}{\beta\gamma} \right) \rho \right] \tag{3}$$

$$= \frac{\vec{\nabla} \cdot \left[-\rho \vec{F}_{\text{ext}} + \rho \vec{\nabla} V(\vec{x};\lambda) + \beta^{-1} \vec{\nabla} \rho \ \right]}{\gamma} \tag{4}$$

By setting $\vec{F}_{\text{ext}}$ to zero, we recover the steady state solution, namely equilibrium distribution ρ_{eq} from Equation 1.

Now suppose that the control parameters $\lambda(t)$ is time dependent. Subsequently, so is now the potential V, i.e. $\partial_t V \neq 0$. As was phrased in the introduction, we want to solve for $\vec{F}_{\text{ext}}(t)$ that offsets the non-adiabatic perturbations, namely, so that $\rho(x;\lambda(t)) = \rho_{\text{eq}}(x;\lambda(t))$

Using now the relations:

$$\vec{\nabla} \rho_{\text{eq}} = -\beta \rho_{\text{eq}} \vec{\nabla} V(x;\lambda)$$

we arrive to the relation by plugging in the Boltzmann distribution (Eq. 1) to the Fokker-Planck solution (Eq. 3):

$$-\gamma \partial_t \rho_{\text{eq}} = \vec{\nabla} \cdot \left(\rho_{\text{eq}} \ \vec{F}_{\text{ext}} - \rho_{\text{eq}} \vec{\nabla} V(\vec{x};\lambda) - \beta^{-1} \vec{\nabla} \rho_{\text{eq}} \right) \tag{5}$$

$$= \vec{\nabla} \cdot \left[\rho_{\text{eq}} \ \vec{F}_{\text{ext}} - \rho_{\text{eq}} \vec{\nabla} V(\vec{x};\lambda) - \beta^{-1} (-\beta \rho_{\text{eq}} \vec{\nabla} V(x;\lambda)) \right] \tag{6}$$

$$= \vec{\nabla} \cdot \left[\rho_{\text{eq}} \ \vec{F}_{\text{ext}} \right] \tag{7}$$

Defining know:

$$\vec{P} := \rho_{\text{eq}} \ \vec{F}_{\text{ext}} \tag{8}$$

we now have:

$$\nabla \cdot \vec{P} = -\gamma \partial_t \rho_{\text{eq}} \tag{9}$$

wherein we rewrote $Z(\lambda)$ and $V(x;\lambda)$ as Z_λ and $V_\lambda(x)$ respectively as to compacti-fy things. Equation 9 is the governing equation of ESE. In previous works, it has been solved in one dimension [cite]. In this paper, we will generalize this result to (1) higher dimesional spaces, and (2) abritrary, non-Euclidean manifolds.

III. SOLUTION VIA THE HODGE DECOMPOSITION

Consider that our phase space is no longer $\mathbb{R}^d$, but rather an arbitrary compact, orientable Riemannian

* Equal Contribution

manifold M with metric g. Re-writing now the vector $\vec{P}$ as a differential one-form $P = P_i dx^i$, we can rewrite equation 9 as:

$$d^\dagger P = \gamma\dot{\lambda}\partial_\lambda\big(\ln[Z_\lambda] + \beta V_\lambda(x)\big)\rho_{\text{eq}} \tag{10}$$

whereby $d^\dagger$ is the Hodge-dual exterior derivative operator.

Because the right hand side of Eq. 10 is equal to $-\gamma\partial_t\rho_{\text{eq}}$, we have by the conservation of probability flow:

$$\int_M -\gamma\frac{\partial}{\partial t}\rho_{\text{eq}}\ dV = -\gamma\frac{\partial}{\partial t}\int_M \rho_{\text{eq}}\ dV = 0 \tag{11}$$

The Hodge Decomposition states that, for any k-form P_k on a compact, orientable Riemannian manifold M, there exists a unique decomposition:

$$P_k = dA_{(k-1)} + d^\dagger B_{(k+1)} + C_k \tag{12}$$

whereby d and $d^\dagger$ are respectively the exterior derivative and its Hodge dual, A_{k-1} and B_{k+1} are $(k-1)$- and $(k+1)$-forms, and C_k is a harmonic k-form (i.e. $\Delta\gamma = 0$, where $\Delta = dd^\gamma + d^\gamma d$, the generalized Laplacian operator).

We plug our $k = 1$-form P into Eq. (i.e. $P = \omega_{k=1}$, and apply d^γ to both sides to get:

$$\begin{aligned} d^\dagger P &= d^\dagger(dA + d^\dagger B + C) \\ &= d^\dagger dA + d^\dagger C \\ &= \Delta A + d^\dagger C \end{aligned}$$

wherein A is a 0-form scalar, and γ is a harmonic one-form. To get the second, we use $d^\dagger d^\dagger = 0$, and to get the third, we use $d(d^\dagger d\alpha_0) = d(0)$, as the exterior derivative of a constant/scalar zero-form is 0. We will see that a general solution exists upon setting $B, C = 0$. (why is this the case?), to finally get:

We are now left with:

$$\Delta A = -\gamma\partial\rho_{\text{eq}} \tag{13}$$

wherein Δ is the Generalized Laplacian operator $d^\dagger d + dd^\dagger$.

Quick note: because B vanishes, we can easily add/subtract it, so in a way we may change gauges by setting $B \neq 0$, and therefore making the substitution $P \leftarrow P - d^\dagger B$. (Remember that $P = \rho_{\text{eq}}F_{\text{ext}}$!)

IV. EXAMPLES

A. Higher Dimensional Euclidean Space

To be written.

B. Rigid Rotor

Lettuce now consider a rigid rotor, whose phase space is the two dimensional sphere $M = S^2$. We have

$$\Delta A = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial A}{\partial\theta}\right) + \frac{\partial^2 A}{\partial\phi^2} \tag{14}$$

There exists a very-good eigenbasis for this operator in S^2, namely the spherical harmonics $\{Y_l^m(\theta,\phi)\}$, which we use in solving Equation 13.

A simple example is to consider an electric dipole with dipole moment p sitting in a time-varying electrical field pointed in the z-direction $\vec{E} = E(t)\hat{z}$, which corresponds to the potential:

$$V(\theta,\phi,t) = -pE(t)\cos(\theta) \tag{15}$$

Because there is no ϕ dependence, the spherical harmonics reduce to the Lengendre polynomials $P_l(\cos\theta)$. This is supposed to be a Big-O.

Given the higher-temperature regime where $\beta^{-1} = k_B T >> |pE(t)|$, we can approximate the Boltzmann distribution:

$$\begin{aligned} \rho(\theta,\phi,t) &\approx \frac{1 - \beta V(\theta,\phi,t)}{4\pi} \\ &\approx \frac{1 + (\beta pE(t)\cos\theta)}{4\pi} \end{aligned}$$

whereby we use that for this particular particular potential, $Z = 4\pi + \mathbb{O}((\beta|pE(t)|)^2)$. that's right, this is supposed to be a big-O notation.

We plug now everything into for Equation 13:

$$\Delta A = -\frac{\gamma\beta p\dot{E}(t)}{4\pi}\cos\theta \tag{16}$$

and we identify the right hand side as with the $l = 1$ Lengendre polynomial, i.e. $P_{l=1}(\cos\theta) = \cos\theta$. Given that $\Delta P_l(\cos\theta) = -l(l+1)P_l(\cos\theta)$, we immediately get:

$$A(t) = \frac{\gamma\beta p\dot{E}(t)}{8\pi}\cos\theta \tag{17}$$

To invert to get back $\vec{F}_{\text{ext}}(t)$, we remember that $\vec{P} = \vec{\nabla}A$, and that $\vec{F}_{\text{ext}} = \vec{P}/\rho_{\text{eq}}$

$$\vec{F}_{\text{ext}} = \frac{\vec{\nabla}A}{\rho_{\text{eq}}} \tag{18}$$

$$\approx \frac{\gamma\beta p\dot{E}(t)}{2}\sin(\theta)\ \hat{\theta} \tag{19}$$

which is enforceable by adding an external electric field $\Delta E_{\text{ESE}}(t) = \gamma\beta\dot{E}/2$.

Intriguingly, if the original time-changing potential were a sinusoid, for instance $E(t) = E_0\cos(\omega t)$, the ESE perturbation correction, to first order, would be to modulate the original signal with an exactly out-of-phase contribution to the original field, $\Delta E_{\rm ESE}(t) = -(\gamma\beta\omega/2)E_0\sin(\omega t)$.

The resulting electric field would then be $E_{\rm net}(t) = AE_0 cos(\omega t+\phi)$, where $A = \sqrt{1+(\gamma\beta\omega/2)^2}$, and $\phi = \tan^{-1}(\gamma\beta\omega/2)$ – a phase-shifted sinusoid from the original electric field.

In other words, to recover the equilibrium probability distribution for a sinusoidal electric field, you would apply a net electric field of the same frequency, but just phase-shifted in time, and with a slightly larger amplitude. The larger the sinusoidal frequency, the larger the phase- and ampitude-shifts.

C. Pair o' Pendula

The last example we will pursue is that of a Pair o' pendula, see Figure (draw a sketch of a pair of pendula).

$$\begin{aligned} V(\theta_1,\theta_2,t) &= ... \\ &- g_1\cos\left(\theta_1\right) - g_2\cos(\theta_2-\phi(t)) - \kappa(t)\cos(\theta_1-\theta_2) \end{aligned}$$

wherein we have the control parameters $\phi(t)$ and $\kappa(t)$, representing the θ_2 bias and θ_1-θ_2 coupling terms respectivly.

We will consider two limits: high temperature, i.e. $\beta^{-1} >> \min(g_1,g_2,\kappa)$, and low temperature: $\beta^{-1} << \max(g_1,g_2,\kappa)$.

For high temperature, we have that $Z(\phi,\kappa) \approx (2\pi)^2$ (to first order), and that:

$$\rho_{\rm eq}(\theta_1,\theta_2,t) \approx \frac{1-\beta V(\theta_1,\theta_2,t)}{4\pi^2}$$

We have then the equation to solve:

$$\begin{aligned} \Delta A &\approx \left(\frac{\gamma\beta}{4\pi^2}\right)\frac{\partial V(\theta_1,\theta_2,t)}{\partial t} \\ &= \left(\frac{\gamma\beta}{4\pi^2}\right)[g_2\dot\phi\sin(\theta_2-\phi) - \dot\kappa\cos(\theta_2-\theta_1)] \end{aligned}$$

Considering the 2-d Fourier basis $f_{k_m,k_n}(\theta_1,\theta_2) = \cos(k_m\theta_1+k_n\theta_2+\phi)$, we have $\Delta f_{k_m,k_n}(\theta_1,\theta_2) = -(k_m^2+k_n^2)f_{k_m,k_n}(\theta_1,\theta_2)$

We have then:

$$A(t) = \left(\frac{\gamma\beta}{4\pi^2}\right)[-g_2\dot\phi\sin(\theta_2-\phi) + \frac{\dot\kappa}{2}\cos(\theta_2-\theta_1)] \quad (20)$$

Solving for $\vec F_{\rm ext}$, we have:

$$\begin{aligned} \vec F_{\rm ext} &= \frac{\vec\nabla A}{\rho_{\rm eq}} \\ &= \gamma\beta(\frac{\dot\kappa}{2}\sin(\theta_2-\theta_1)(\hat\theta_1-\hat\theta_2) - g_2\dot\phi\cos(\theta_2-\phi)\hat\theta_2) \end{aligned}$$

This is more or less the high temperature case. For the low temperature case, we use the second order cos approximation, assuming that is only those terms that would dominate in $\exp(-\beta V)$:

$$\begin{aligned} -\beta V &\approx \beta g_1(1-\frac{\theta_1^2}{2}) + \beta g_2(1-\frac{(\theta_2-\phi)^2}{2}) + \kappa(1-\frac{(\theta_2-\theta_1)^2}{2}) \\ &= \beta(g_1+g_2+\kappa) + ... \\ &\frac{\beta}{2}(g_1\theta_1^2 + g_2(\theta_2^2-2\theta_2\phi+\phi^2) + \kappa(\theta_2^2-2\theta_2\theta_1+\theta_1^2)) \end{aligned}$$

Adrianne: I am struggling to finish this part. Original idea, the sum of quadratics (in 2 variables) is still a quadratic, after taking the exponent we would have then a 2d Gaussian. However, it is largely possible that the case the center of the Gaussian, $(\bar\theta_1,\bar\theta_2)$ is far away from where the 2nd order approximation of cosine holds (ie $\theta_1, \theta_2-\phi, \theta_1-\theta_2 << 1$, for certain parameter choices of ϕ.

Best to try to solve analytically the integral $\exp(\beta(\cos(\theta_1)+\cos(\theta_2-\phi)+\kappa(\theta_2-\theta_1))$