SUB-RIEMANNIAN GEOMETRY AND FINITE TIME THERMODYNAMICS PART 1: THE STOCHASTIC OSCILLATOR

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Abstract. The field of sub-Riemannian geometry has flourished in the past four decades through the strong interactions between problems arising in applied science (in areas such as robotics) and questions of a pure mathematical character about the nature of space. Methods of control theory, such as controllability properties determined by Lie brackets of vector fields, the Hamilton equations associated to the Maximum Principle of optimal control, Hamilton-Jacobi-Bellman equation etc. have all been found to be basic tools for answering such questions. In this paper, we find a useful role for the vantage point of sub-Riemannian geometry in attacking a problem of interest in non-equilibrium statistical mechanics: how does one create rules for operation of micro- and nano-scale systems (heat engines) that are subject to fluctuations from the surroundings, so as to be able to do useful things such as converting heat into work over a cycle of operation? We exploit geometric optimal control theory to produce such rules selected for maximal efficiency. This is done by working concretely with a model problem, the stochastic oscillator. Essential to our work is a separation of time scales used with great efficacy by physicists and justified in the linear response regime.

1. Introduction. Sub-Riemannian geometry has roots in optimal control problems [6] [7]. The essential connectivity theorem for this setting, the Chow-Rashevskii theorem on accessibility [15] [32] [19], also brings the subject into contact with an axiomatic approach to macroscopic thermodynamics, initiated by Carathéodory [12] (with encouragement from Max Born as noted in [5]). The Carathéodory principle that “existence of states inaccessible by adiabatic process from every state” is equivalent to the existence of an integrating factor – absolute temperature, contains the essence of the second law of thermodynamics (see discussion in chapter 1 of [13], and chapter 22 of [3]). The penetrating insights of Gromov [17] [18] direct one to other roots of the field of sub-Riemannian geometry based on exploration of length structures. For further historical remarks and perspectives see also the Mathematical Reviews article [25] of Montgomery on [17], and [26]. Pioneering investigations in a control-theoretic spirit into macroscopic thermodynamic engines by Brockett and Willems [10], and Brockett [8] [9], have centered on equilibrium statistical physics. For instance the Nyquist-Johnson resistor model coupled to a quasi-statically controllable capacitance was the focus of [10] and resulted in a Carnot cycle calculation using moment analysis of linear stochastic differential equations. We too are guided...
by similar questions of thermodynamic engines, but on a microscopic scale, where fluctuations matter and are used to extract work from a heat bath by manipulating system parameters in cycles of finite duration. This is a setting of non-equilibrium statistical physics, dissipation must be taken into account, and cycles of maximum efficiency are of interest. We work out this program for a concrete physical problem, focusing on a linear oscillator of controllable stiffness in contact with a heat bath at controllable temperature. This physical setting has been investigated previously by Sivak and Crooks [33] and Zulkowski, Sivak, Crooks and DeWeese [36], motivated by its relevance to biophysical experiments with laser traps holding beads attached to polymer molecules (see figure 1). They demonstrate that approximations relevant in the linear response regime [37] yield novel calculations of dissipation and associated Riemannian geometry. A contribution of the present work is to show that out of this emerges sub-Riemannian geometry of contact type [2] and the problem of maximum efficiency cycles is an optimal control problem best tackled by methods natural to this context.

In what follows we discuss the structure of the paper. In Section II of the paper, the model problem of a heat engine, a parametrically controlled stochastic oscillator, is examined as a dissipative system, and in the system-theoretic language of Willems [34], a (unitless) storage function and supply rate are identified. Further an average dissipation rate is determined, first abstractly, and then more explicitly as a quadratic form on the tangent space of the system parameter manifold. This positive definite inverse diffusion tensor, the end-product of appealing to linear response approximation, justified as in Appendix A by a separation of time scales, gives a Riemannian structure on parameter manifold [36]. The system parameter space together with the work extracted from the bath constitutes a sub-Riemannian space with an associated deterministic controllable system with 2 controls. This is the culmination of taking averages to pass from the time scale of fluctuations to the slower time scale of the heat engine. Section III presents a formula for efficiency of the heat engine for any protocol (i.e. path in parameter space) generated by the deterministic control system derived in section II. This is the basis for our main theorem 3.1 – maximizing efficiency is generically equivalent to minimizing dissipation subject to prescribed extracted work in a cycle of the engine. This optimal control problem is then analyzed using the maximum principle of control theory to derive necessary conditions (Hamilton’s equations) [1] [2] [4] [21], followed by reduction to dynamics on level set of the Hamiltonian. Then a characterization of true minimizers is given via conjugate point theorem 3.5. Section IV is concerned with numerical design of cycles in system parameter space using the level set method to solve the sufficient conditions for optimality – the Hamilton-Jacobi-Bellman partial differential equation governing the optimal dissipation function (or value function in common control-theoretic terminology). A set of designs is derived, using a combination of hand-crafted and public domain codes for this purpose. Appendix B provides some key steps that lead to scaling between time duration of an optimal path in parameter space, arc length of an optimal curve, and the associated Hamilton-Jacobi equation to be solved as laid out in the Osher theory [29]. All numerical calculations are done according nominal parameters for the stochastic oscillator as in Appendix C, and convenient re-scaling for proper conditioning.

2. Dissipation and inverse diffusion tensor. A heat engine is a cyclically operated statistical mechanical system which generates net mechanical work per cycle
using heat supply from a heat bath. As it is operated in finite-time, this non-equilibrium statistical mechanical system is a dissipative system. In this paper, we model such an engine by a stochastic oscillator, specifically a linear oscillator in contact with a heat bath. In nano-scale systems research, the stochastic oscillator can be implemented by a bead in an optical trap as shown in figure 1.

**Figure 1.** Bead-in-trap illustration: (a) realization of stochastic oscillator – an optical trap is deployed by focusing a laser beam with the objective lens. Due to the transfer of momentum from the scattering of incident photons, a colloidal bead near the trap focus will experience a force. When the bead is under stable trapping, the force can be approximated as a gradient force which is in the direction of the spatial light gradient. It is proportional to the optical intensity at the focus and pulls the particle towards the focal region. If the bead is at small displacement away from the focus, the gradient force is also proportional to the displacement. Thus, a bead-in-trap system can be modeled as a spring-mass system. As the bead in the optical trap is immersed in a fluid and is subject to fluctuation (Brownian motion), the optical trap system can be viewed as a heat bath. The temperature of the solution and the stiffness of the potential well (governed by the intensities of the beams) are two controllable parameters. (text adapted from [27])

(b) apparatus for biophysical measurement – in the famous experiment [11] [23] to verify the Jarzynski equality [20], an optical trap is deployed to measure the force exerted on a molecule of RNA which connects two beads. The RNA is subject to irreversible and reversible cycles of folding and unfolding. The actuator controls the position of the right bead and it will stretch the RNA. The optical trap will determine the force exerted on the molecule. The distance between the beads is the end-to-end length of the molecule. The length of the molecule and the exerted force on the molecule give the measurement of the work done on the molecule along different stochastic trajectories which is the essence of the experiment. (text and figure adapted from [11])
2.1. A Hamiltonian system in contact with a heat bath. A stochastic oscillator with position $\xi_1$ and momentum $\xi_2$ is driven by Brownian motion,

$$d\xi_1 = \frac{\xi_2}{m} dt$$
$$d\xi_2 = -\frac{\zeta \xi_2}{m} dt - k\xi_1 dt + \sqrt{\frac{2\zeta}{\beta}} dB(t)$$

where $B(t)$ is standard Brownian motion, such that the averages

$$\langle dB(t) \rangle = 0$$
$$\langle dB(t) dB(t') \rangle = \delta(t - t') dt'$$

We let $\xi = (\xi_1, \xi_2)$ denote the state of the oscillator. Angled brackets indicate statistical average of Brownian motion and $\delta$ is Dirac delta function. $\zeta$ is the Cartesian friction constant (determined by the shape of the bead and fluid viscosity; for spherical beads it is given by a formula due to Stokes [31]). At time $t$, $\beta(t) = (k_B T)^{-1}$ is the inverse temperature of the heat bath in natural units with Boltzmann constant $k_B$ and $k(t)$ is the stiffness of the potential well. The pair $\lambda = (\beta, k)$ is the system parameter, and a protocol $\Lambda$ is a time-dependent path of $\lambda$.

The stochastic oscillator in contact with a heat bath is a special case of a Hamiltonian system in contact with a heat bath,

$$d\xi = (J - G) \frac{\partial H(\xi, \lambda)}{\partial \xi} dt + \sqrt{\frac{2}{\beta}} G^{1/2} dw_t.$$  

In (3), $\xi$ is the $d$-dimensional state variable and $\omega_t$ denotes an $\mathbb{R}^d$-valued Wiener-process while $J$ is a skew-symmetric matrix ($J = -J^T$) and $G$ is a $d$-dimensional positive-semidefinite matrix, such that

$$G = \begin{pmatrix} 0 & 0 \\ 0 & \tilde{G} \end{pmatrix}$$

where $\tilde{G}$ is a positive-definite matrix ($\tilde{G} = \tilde{G}_1 \tilde{G}_1^T$) and the dimension of $\tilde{G}$ is less than or equal to $d$. In the case that the dimension of $\tilde{G}$ is less than $d$, $G^{1/2}$ is

$$\begin{pmatrix} 0 & 0 \\ 0 & \tilde{G}_1 \end{pmatrix}.$$  

In the stochastic oscillator, $d = 2$ and

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$
$$G = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$  

As a dissipative dynamical system [34], we consider the unitless term $S = \beta H$ as the storage function, where $H$ is the Hamiltonian of the system which is a function of the state $\xi$ and the system parameter $\lambda$. Correspondingly, the vector $\dot{\lambda}$ is the input, $X = \frac{\partial S}{\partial \lambda}$ is the output and $w = \dot{\lambda}^T X$ is the supply rate. For a statistical mechanical system, its state probability density at equilibrium

$$\rho_{eq,\lambda}(\xi) \propto e^{-\beta H}$$

when the system is held at fixed control parameter $\lambda$. For us, dissipativeness has to do with transition of a system which has been disturbed from equilibrium to a new equilibrium. When $\lambda$ is changed to a new value, the oscillator undergoes a transition to a new equilibrium probability distribution. In general this process results in dissipation of energy.

We define the average dissipation rate (in the spirit of [34])

$$d = \langle w \rangle - \frac{d}{dt} \langle S \rangle_{eq,\lambda},$$

where $\langle \rangle$ is the average evaluated with non-equilibrium distribution (obtained by solving the Fokker-Planck equation with time dependent coefficients [31] associated
to the stochastic dynamics) and $\langle \cdot \rangle_{eq, \lambda}$ is the average evaluated with the equilibrium distribution of the statistical mechanical system with system parameter $\lambda$. For the stochastic oscillator, the Hamiltonian $H(\xi, \lambda) = \frac{\xi^2}{2m} + \frac{k\xi^2}{2}$ is the total energy. Given that $S(t, \xi) \in C^2([0, \infty) \times \mathbb{R}^2)$, by Ito's formula [30],

$$
\frac{dS}{dt} = \left( \frac{\partial S}{\partial \xi_1} \right) d\xi_1 + \left( \frac{\partial S}{\partial \xi_2} \right) d\xi_2 + \frac{1}{2} \text{tr} \left( \left( \frac{\partial^2 S}{\partial \xi_1 \partial \xi_1} \right) \left( \left( \frac{0}{\sqrt{2\beta}} \right) \right) \left( \frac{0}{\sqrt{2\beta}} \right) \right) dt
$$

(7)

By the equipartition theorem [31], $\langle \frac{k\xi^2}{2} \rangle_{eq, \lambda} = \langle \xi^2 \rangle_{eq, \lambda} = \frac{1}{2\beta}$ and

$$
\frac{d}{dt} \langle S \rangle_{eq, \lambda} = \dot{\lambda}^T \langle X \rangle_{eq, \lambda} = \frac{\dot{\beta}}{\beta} + \frac{k}{2\beta}.
$$

(8)

Thus,

$$
d = \dot{\lambda}^T (X - \langle X \rangle_{eq, \lambda}) = \dot{\lambda}^T (\Delta X)
$$

(9)

where the vector $\Delta X \equiv X - \langle X \rangle_{eq, \lambda}$.

The average dissipation rate defined above is closely related to the energy dissipation rate in non-equilibrium statistical mechanics. For the stochastic oscillator, the equilibrium distribution is Boltzmann distribution, $\rho_{eq, \lambda}(\xi) = \frac{e^{-\beta H(\xi, \lambda)}}{Z(\lambda)}$, where $Z(\lambda) \equiv \int e^{-\beta H(\xi, \lambda)} d\xi$ is the partition function. Moreover,

$$
- \frac{\partial \ln \rho_{eq, \lambda}}{\partial \lambda} = \Delta X.
$$

(10)

The thermodynamical entropy associated to $\rho$ is

$$
\mathcal{H}(\rho) = -k_B \int \rho(\xi) \ln \rho(\xi) d\xi.
$$

(11)

The internal energy $U$ of the system is the average value of the total energy $H(\xi, \lambda)$ which is denoted below as $U_{neq}$ when it is evaluated with non-equilibrium distribution. Free energy

$$
F = U - T\mathcal{H}
$$

(12)

is the portion of internal energy which could be converted to mechanical work or dissipated into surrounding environment. At equilibrium,

$$
F_{eq} = -k_B T \ln Z(\lambda)
$$

(13)

For a non-equilibrium distribution $\rho_{neq, \lambda}$ with a time-dependent protocol $\lambda(t)$, its divergence from the equilibrium distribution with the same system parameter is measured by relative entropy $D(\rho_{neq, \lambda} \| \rho_{eq, \lambda}) = \int \rho_{neq, \lambda} \ln \left( \frac{\rho_{neq, \lambda}}{\rho_{eq, \lambda}} \right) d\xi$ and
\[
D(\rho_{\text{neq} \lambda} \| \rho_{\text{eq} \lambda}) = \int \rho_{\text{neq} \lambda} \ln \rho_{\text{neq} \lambda} d\xi - \int \rho_{\text{eq} \lambda} \ln \rho_{\text{eq} \lambda} d\xi
= -\frac{1}{k_B} \mathcal{H}(\rho_{\text{neq} \lambda}) - \int \rho_{\text{neq} \lambda} \ln \frac{e^{-\beta H(\xi, \lambda)}}{Z(\lambda)} d\xi
= -\frac{1}{k_B} \mathcal{H}(\rho_{\text{neq} \lambda}) + \beta U_{\text{neq}} - \beta F_{\text{eq}}
= \beta (F_{\text{neq}} - F_{\text{eq}}). \tag{14}
\]

As relative entropy is non-negative, in relaxing from non-equilibrium to equilibrium under the Fokker-Planck dynamics, the statistical mechanical system dumps (part of) its free energy to surroundings. In the case of the stochastic oscillator, the energy dissipation refers to the (unitless) loss of free energy. Thus, the time derivative of relative entropy is the energy dissipation rate of the system:

\[
\frac{d}{dt} D(\rho_{\text{neq} \lambda} \| \rho_{\text{eq} \lambda}) = \int \frac{\partial \rho_{\text{neq} \lambda}}{\partial t} \ln \left( \frac{\rho_{\text{neq} \lambda}}{\rho_{\text{eq} \lambda}} \right) d\xi
+ \int \rho_{\text{neq} \lambda} \left( \frac{1}{\rho_{\text{eq} \lambda}} \frac{\partial \rho_{\text{neq} \lambda}}{\partial t} - \frac{\partial \ln \rho_{\text{eq} \lambda}}{\partial t} \right) d\xi \tag{15}
= \int \frac{\partial \rho_{\text{neq} \lambda}}{\partial t} \ln \left( \frac{\rho_{\text{neq} \lambda}}{\rho_{\text{eq} \lambda}} \right) d\xi + \dot{\lambda}^\tau \langle \Delta X \rangle.
\]

On the right hand side of above equality, the first term in the case of stochastic oscillator [35] can be simplified as

\[
-\frac{\zeta}{\beta} \int e^{-\frac{\rho_{\text{neq}}}{m}} \left[ \frac{1}{\rho_{\text{neq}}} \left( \frac{\partial}{\partial \xi_2} \left( \frac{\rho_{\text{neq}}}{\rho_{\text{eq}}} \right)^2 \right) \right] \leq 0 \tag{16}
\]

and the second term is the average dissipation rate \( d \). Therefore, \( d \) is an upper bound of the energy dissipation rate.

2.2. Inverse diffusion tensor of a stochastic oscillator. The average dissipation rate is \( d = \dot{\lambda}^\tau \langle \Delta X \rangle \). To analyze the average dissipation rate \( d \), it is crucial to compute an expression for \( \langle \Delta X \rangle \). Assuming that \( \lambda \) is varied smoothly and the statistical mechanical system is always near its equilibrium, linear response theory is the standard framework for understanding \( \langle \Delta X \rangle \) [37]. The discussion in this subsection is mainly as stated in [35] and [33] and it is presented with greater detail in Appendix A.

Based on the calculation in [36], in the space of system parameter \( \lambda = (\beta, k) \), the inverse diffusion tensor of the stochastic oscillator has constant negative Ricci curvature \(-2\zeta/m\). The ranges of \( k \) and \( \beta \) are both positive. By a theorem from Riemannian geometry [16], there is an isometric mapping between this constant negative-curvature submanifold and a submanifold of Poincaré upper half plane:

\[
x = \frac{1}{4\beta k}, \quad y = \frac{1}{2\beta \zeta} \sqrt{\frac{m}{k}}
\]

\[
d = \frac{m \dot{x}^2 + \dot{y}^2}{\zeta \dot{y}^2} \tag{17}
\]

The dissipation rate in the unit \((k_B T/\text{sec})\) in space \((x, y)\)

\[
\tilde{d} = \frac{d}{\beta} = \zeta \left( \frac{\dot{x}^2 + \dot{y}^2}{x} \right) = \left( \begin{array}{c} \dot{x} \\ \dot{y} \end{array} \right) \left( \begin{array}{cc} \zeta & 0 \\ 0 & \frac{1}{\zeta} \end{array} \right) \left( \begin{array}{c} \dot{x} \\ \dot{y} \end{array} \right). \tag{18}
\]
This positive-definite tensor \( \begin{pmatrix} \frac{\zeta}{x} & 0 \\ 0 & \frac{\zeta}{y} \end{pmatrix} \) can be viewed as a metric tensor \( g[\lambda] \) in the space of \((x, y)\). The geometric energy of a curve in \((x, y)\) space has the statistical mechanical meaning of the energy dissipation while following a protocol.

**Remark 1.** In our example of the stochastic oscillator, note that the average dissipation rate \( \dot{d} \) has a positive-definite inverse diffusion tensor. Indeed, it is a dissipative dynamical system in the spirit of [34].

2.3. **Subriemannian geometry of a heat engine.** Besides the dissipation of energy in the analysis of non-equilibrium thermodynamic system, there are auxiliary quantities of interest, such as the average extracted work \( \psi \) of a heat engine, which is a functional of a protocol. The system parameter space \( M \) is enlarged to a higher dimensional manifold \( N \) of pairs \((\lambda, \psi)\). Let \( \pi \) denote the projection from \( N \) to \( M \). Since \( \pi \) is a surjective submersion, \( \pi^{\ast} \) is the corresponding push-forward action \( \pi^{\ast} : T_{(\lambda, \psi)}N \rightarrow T_{\lambda}M. \) \( \pi^{\ast} \) and metric tensor \( g \) on \( M \) induce a positive semidefinite inner product \( \langle \cdot, \cdot \rangle_{N} \) on the manifold \( N \).

\[
\forall v_1, v_2 \in T_{(\lambda, \psi)}N, \quad \langle v_1, v_2 \rangle_N = g(\pi^{\ast}v_1, \pi^{\ast}v_2) \tag{19}
\]

It follows, as the number of control variables is smaller than the dimension of \( T_{(\lambda, \psi)}N \), we ask if a sub-Riemannian manifold structure might exist in the space \( N \). This requires controllability. Once we write down the protocol dynamics explicitly, as a control system, controllability is characterized by the Chow-Rashevskii theorem [1] [15] [26] [32].

At time \( t \), the mechanical power \( \dot{\psi} \) is extracted from the oscillator by varying the stiffness of potential well during the transition between equilibrium states and

\[
\dot{\psi} = \left\langle \frac{\partial}{\partial k} \left( \frac{\zeta k^2}{x^2} \right), k \right\rangle_{eq, \lambda} = \frac{\zeta^2}{m} \left( \frac{y^2}{x^2} \ddot{x} - \frac{y}{x} \ddot{y} \right). \tag{20}
\]

In linear response regime, the average dissipation rate \( \bar{d} \) of the heat engine is positive while the system parameter of the engine is varied, and is given in the unit of \( k_B T/\text{sec} \) as

\[
\bar{d} = \frac{\zeta(\dot{x}^2 + \dot{y}^2)}{x}. \tag{21}
\]

which defines the metric tensor on the system parameter manifold of \((x, y)\). Now \((\sqrt{\frac{\zeta}{x}}, 0)^T\) and \((0, \sqrt{\frac{\zeta}{y}})^T\) are orthonormal vectors on the tangent space to the system parameter manifold. The dynamics of the heat engine can now be formulated as a deterministic control system,

\[
\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{\psi} \end{pmatrix} = u \begin{pmatrix} \sqrt{\frac{\zeta}{x}} \\ 0 \\ \zeta^{3/2} \end{pmatrix} + v \begin{pmatrix} 0 \\ \sqrt{\frac{\zeta}{y}} \\ -\zeta^{3/2} \end{pmatrix} \tag{22}
\]

where \( u \) and \( v \) now take the role of control signals, generating the protocol.

Letting \( m \) and \( \zeta \) be unity in the controllability analysis, for the vector fields \( f_1 = (\sqrt{x}, 0, \frac{\sqrt{\zeta}}{x})^T \) and \( f_2 = (0, \sqrt{x}, -\frac{y}{x})^T \), the Lie bracket \([.,.]\) of \( f_1 \) and \( f_2 \) gives \( f_3 = [f_1, f_2] = (0, \frac{1}{x}, -\frac{3y}{2x})^T \). The rank \([f_1, f_2, f_3] = 3\) indicates that the system \( (22) \) is controllable (completely nonholonomic). From above definitions, it follows that
\[ d = u^2 + v^2 \] and hence, the problem finding a protocol minimizing dissipation is an optimal control problem for (22) with quadratic cost functional.

3. Design of a heat engine with maximum efficiency. As a heat engine, under certain operating conditions, can extract heat from its heat bath to output mechanical work, it is essential to define the extracted work of the engine and the total heat supply from heat bath to it for efficiency analysis of the heat engine. For our stochastic oscillator, these quantities will be defined as the basis for later investigation of efficiency of the heat engine. For the stochastic oscillator with dynamics (1), given that its internal energy \( U_{\text{neq}} \) is the average value of

\[ H = \frac{k\xi_1^2}{2} + \frac{\xi_2^2}{2m} \]

by Ito’s rule [30],

\[
\begin{align*}
\dot{H} &= \frac{\partial H}{\partial k} \dot{k} + \frac{\partial H}{\partial \xi_1} d\xi_1 + \frac{\partial H}{\partial \xi_2} d\xi_2 + \frac{1}{2} \text{tr} \left( \left( \frac{\partial^2 H}{\partial \xi_1^2} \right) \left( \frac{\partial^2 H}{\partial \xi_2^2} \right) \right) \left( 0 \ 0 \ 0 \ \frac{\zeta}{\beta} \right) dt \\
&= \frac{\dot{k}\xi_1^2}{2} dt - \zeta \frac{\xi_2^2}{m^2} dt + \frac{\xi_2}{m} \sqrt{\frac{2\zeta}{\beta}} dB(t) + \frac{\zeta}{m\beta} dt.
\end{align*}
\]

Taking average on both sides of above equation,

\[
\dot{U}_{\text{neq}} = \left\langle \frac{\dot{k}\xi_1^2}{2} \right\rangle - \left\langle \zeta \frac{\xi_2^2}{m^2} \right\rangle + \frac{\zeta}{m\beta}
\]

where \( \dot{U}_{\text{neq}} \) is the rate of change of the internal energy, \( -\left\langle \frac{\dot{k}\xi_1^2}{2} \right\rangle \) is the extracted mechanical power of the stochastic oscillator. In consequence, from time 0 to time \( t_f \), the integral \( \int_0^{t_f} \left\langle \dot{k}\xi_1^2 \right\rangle \) is the extracted work of the stochastic oscillator. The difference between the fluctuation and dissipation \( \frac{\zeta}{m\beta} - \left\langle \zeta \frac{\xi_2^2}{m^2} \right\rangle = \dot{U}_{\text{neq}} - \left\langle \frac{\dot{k}\xi_1^2}{2} \right\rangle \) is the heat flux associated with the heat bath. If it is positive, the heat flux is injected from the heat bath to the engine. If it is negative, the heat flux is from the engine to the heat bath. Thus, using an indicator function \( 1 \), the integral of the positive heat flux from time 0 to time \( t_f \)

\[
\int_0^{t_f} \left( \dot{U}_{\text{neq}} - \left\langle \frac{\dot{k}\xi_1^2}{2} \right\rangle \right) 1 \left\{ \dot{U}_{\text{neq}} - \left\langle \frac{\dot{k}\xi_1^2}{2} \right\rangle > 0 \right\} dt
\]

is the heat supply from the heat bath to the engine. If we approximate the integrands inside above two integrals with equilibrium averages \( \langle U_{\text{eq,}\lambda} = \frac{1}{\beta} \) and \( \langle \frac{k\xi_1^2}{2} \rangle_{\text{eq,}\lambda} = \frac{1}{\beta^2} \) in the near-equilibrium regime, we see that

\[
\int_0^{t_f} \left( \frac{\dot{k}\xi_1^2}{2} \right)_{\text{eq,}\lambda} dt = \int_0^{t_f} \frac{\dot{k}}{2\beta k} dt
\]

Further, due to the fact that the engine is operated in finite-time, the heat bath will also provide the extra energy dissipated into the surroundings by the engine
which accompanies heat exchange between the engine and the heat bath. The 
\textit{total heat supply} from the heat bath is the sum of the heat supply from the heat bath to the heat engine and the dissipated energy of the heat engine, which in the near-equilibrium regime, approximately equals to

\[
\int_0^{t_f} \left( -\frac{\dot{\beta}}{\beta^2} - \frac{k}{2\beta k} \right) \mathbb{1}\left\{ -\frac{\dot{\beta}}{\beta^2} - \frac{k}{2\beta k} > 0 \right\} + \left( \dot{\beta} \right) g[\lambda] \left( \frac{\dot{\beta}}{k} \right) dt \tag{27}
\]

where \(g[\lambda]\) is the inverse diffusion tensor of the stochastic oscillator at \(\lambda = (\beta, k)\).

3.1. \textbf{Optimal control of the heat engine}. A parametrically-controlled heat engine can convert heat flow (partially) into mechanical work. The engine is modeled by focusing on the control of the system parameter. Based on above discussion, \(\tilde{d} = u^2 + v^2\) is the average dissipation rate in \(k_B T/\text{sec}\). Given a protocol \(\Lambda\), from time \(0\) to time \(t_f\), along a trajectory in the space of \((x,y)\), the total heat supply in the stochastic oscillator system is

\[
\int_0^{t_f} \left( -\frac{\dot{\beta}}{\beta^2} - \frac{k}{2\beta k} \right) \mathbb{1}\left\{ -\frac{\dot{\beta}}{\beta^2} - \frac{k}{2\beta k} > 0 \right\} + \tilde{d} \right) dt. \tag{28}
\]

We express the total heat supply in the coordinate \((x,y)\) as

\[
\int_0^{t_f} \left( \left( \frac{c^2}{m} \frac{\dot{y}}{x} \right) \mathbb{1}\left\{ \frac{\dot{y}}{x} > 0 \right\} + \zeta \left( \frac{x^2 + y^2}{x} \right) \right) dt. \tag{29}
\]

\textbf{Efficiency} \(\eta\) of a heat engine is the ratio of the extracted work of the heat engine to the total heat supply from the heat bath. The efficiency of the stochastic oscillator is

\[
\eta = \frac{\int_0^{t_f} \dot{\psi} dt}{\int_0^{t_f} \left( \left( \frac{c^2}{m} \frac{\dot{y}}{x} \right) \mathbb{1}\left\{ \frac{\dot{y}}{x} > 0 \right\} + \tilde{d} \right) dt}
\]

\[
= \frac{\int_0^{t_f} \left( \frac{c^2}{m} \frac{\dot{y}^2}{x^2} - \frac{\dot{y}}{x} \right) dt}{\int_0^{t_f} \left( \left( \frac{c^2}{m} \frac{\dot{y}}{x} \right) \mathbb{1}\left\{ \frac{\dot{y}}{x} > 0 \right\} + \tilde{d} \right) dt}. \tag{30}
\]

If the extracted work is prescribed, to maximize the efficiency of a heat engine, the total heat supply (i.e. the denominator in \(\eta\)) must be minimized. This can be first formulated as a problem in calculus of variations on the sub-Riemannian manifold \(N\) associated to the stochastic oscillator:

\text{Find } t \rightarrow \gamma(t) = (x(t), y(t), \psi(t)), \text{ a curve on } N \text{ to minimize}

\[
J = \int_0^{t_f} \left( \left( \frac{c^2}{m} \frac{\dot{y}}{x} \right) \mathbb{1}\left\{ \frac{\dot{y}}{x} > 0 \right\} + \tilde{d}_1 \right) dt \tag{31}
\]

such that \(\int_0^{t_f} \dot{\psi} dt\) is a prescribed value and \(x(0), y(0), x(t_f), y(t_f)\) are specified.

As a heat engine is a cyclically operated machine, working loops are a type of protocol of special interest. In the stochastic oscillator, for working loops \(x(0) = x(t_f)\) and \(y(0) = y(t_f)\).

\textbf{Theorem 3.1}. If a non-constant working loop \(\gamma^* \in C^\infty\) is an optimal solution to problem (31) and along \(\gamma^* : [0,t_f] \rightarrow N\), there are a finite number of \(t_i \in [0,t_f](i = 1,2,\ldots,m)\) when \(\frac{\dot{y}}{x}\) is zero (the finiteness hypothesis), then \(\gamma^*\) is also a solution to the following optimal control problem with dynamics (22),
Comparing equations in (36) and (37) at time $t_f$, we must follow Euler-Lagrange equation, such that $\rho \gamma$ where $\rho \gamma$ is the Lagrange multiplier and it is a constant. As an optimal solution, $\gamma_i$ is an equivalent to the integral of $\mathcal{L}$ over $[0, t_f]$, which indicates that the extracted work over $[0, t_f]$ is prescribed value, $(x(0), y(0))$. Suppose during $[t_{0}, t_{1}]$, $\frac{\partial}{\partial x} \gamma$ is a conserved quantity. Similarly, along $\gamma_i$, $\mathcal{L}$ is specified and $\gamma_i \equiv [t_0, t_1] \to N, \ldots, \gamma_i \equiv [t_m, t_{m+1}] \to N$, where we set $t_0 = 0$ and $t_{m+1} = t_f$.

Moreover, as from time 0 to time $t_f$, we have a loop in the parameter space $(x, y)$,

$$\int_0^{t_f} \dot{\psi} dt = \int_0^{t_f} \left( \frac{d}{dt} \beta(x, y) + \dot{\psi} \right) dt = \int_0^{t_f} \frac{\dot{\gamma}}{m} \frac{\dot{y}}{x} dt$$

which indicates that the extracted work over $[0, t_f]$ being a prescribed value is equivalent to the integral of $\frac{\dot{\gamma}}{m} \frac{\dot{y}}{x}$ being the same prescribed value. As $\gamma^*$ is an optimal solution to problem (31) from time 0 to time $t_f$, each $\gamma^*_i : [t_i, t_{i+1}] \to N$ ($i = 0, 1, \ldots, m$) should be optimal for the following problem:

$$\begin{aligned}
\text{Min}_{\gamma_i} \quad J &= \int_{t_i}^{t_{i+1}} \left( \frac{\dot{x}^2}{m} + \frac{\dot{y}^2}{x^2} + 2 \frac{\dot{x}}{x} \right) dt \\
\text{subject to:} \quad \gamma_i(t_i) &= \gamma^*(t_i) \quad \text{and} \quad \gamma_i(t_{i+1}) = \gamma^*(t_{i+1}).
\end{aligned}$$

Suppose during $[t_i, t_{i+1}]$, $\frac{\partial}{\partial x} \gamma$ is non-negative. The augmented Lagrangian along $\gamma^*_i$ is

$$L_i = (1 + \rho_i) \frac{\dot{\gamma}}{m} \frac{\dot{y}}{x} + \frac{x^2 + \dot{y}^2}{x}.$$  (35)

where $\rho_i$ is the Lagrange multiplier and it is a constant. As an optimal solution, $\gamma^*_i$ must follow Euler-Lagrange equation, such that

$$\begin{aligned}
(1 + \rho_i) \frac{\dot{x}^2}{m} + \frac{\dot{y}^2}{x^2} + 2 \frac{\dot{x}}{x} &= 0 \\
(1 + \rho_i) \frac{\dot{y} \dot{x}}{m} - \frac{2 \dot{y}}{x} + \frac{2 \dot{x} \dot{y}}{x^2} &= 0.
\end{aligned}$$  (36)

In time interval $[t_{i+1}, t_{i+2}]$, $\frac{\partial}{\partial x} \gamma$ is either non-negative or non-positive. If $\frac{\partial}{\partial x} \gamma$ is non-negative, it is seen with $\rho_{i+1}$ as the Lagrange multiplier and $L_{i+1}$ as the augmented Lagrangian, $\gamma^*_{i+1}$ should be a solution of following Euler-Lagrange equation

$$\begin{aligned}
(1 + \rho_{i+1}) \frac{\dot{x}^2}{m} + \frac{\dot{y}^2}{x^2} + 2 \frac{\dot{x}}{x} &= 0 \\
(1 + \rho_{i+1}) \frac{\dot{y} \dot{x}}{m} - \frac{2 \dot{y}}{x} + \frac{2 \dot{x} \dot{y}}{x^2} &= 0.
\end{aligned}$$  (37)

Comparing equations in (36) and (37) at time $t_{i+1}$, because of $\gamma^*$'s smoothness,

$$\begin{aligned}
(\rho_i - \rho_{i+1}) \frac{\dot{x} \dot{y}}{x^2} &= 0 \\
(\rho_i - \rho_{i+1}) \frac{\dot{y} \dot{x}}{x} &= 0
\end{aligned}$$  (38)

either $\rho_i = \rho_{i+1}$ or $\dot{x} = 0$ and $\dot{y} = 0$. Note that $L_i$ is time-independent. Along $\gamma^*_i$, $E_i \equiv \frac{\partial^2}{\partial \dot{x}^2} \dot{x} + \frac{\partial^2}{\partial \dot{y}^2} \dot{y} - L_i \equiv \frac{\dot{x}^2 + \dot{y}^2}{x^2}$ is a conserved quantity. Similarly, along $\gamma^*_{i+1}$, $E_{i+1} = \frac{\dot{x}^2 + \dot{y}^2}{x^2}$ is also conserved. If $\dot{x} = 0$ and $\dot{y} = 0$ at time $t_{i+1}$, $E_i$ and $E_{i+1}$ are
both zero along \( \gamma^*_i \) and \( \gamma^*_{i+1} \). Thus, in an interval \([t_i, t_{i+2}]\) we have a static point. If \( t_i = 0 \) and \( t_{i+2} = t_f \), the whole trajectory \( \gamma^* \) is constant, which violates the finiteness hypothesis. The only plausible solution to (38) is \( \rho_i = \rho_{i+1} \).

If \( \frac{3}{2} \dot{y} \) is non-positive from time \( t_{i+1} \) to time \( t_{i+2} \), the augmented Lagrangian is \( \rho_{i+1} \frac{\zeta}{m} x \dot{y} + \zeta \frac{\dot{x}^2 + \dot{y}^2}{x} \) and its Euler-Lagrange equation is

\[
\rho_{i+1} \frac{\zeta}{m} x \dot{y} - \frac{\dot{x}^2}{x} + \frac{\dot{y}^2}{x} + \frac{2 \ddot{x}}{x} = 0
\]

\[
\rho_{i+1} \frac{\zeta}{m} x \dot{y} - \frac{2 \dot{x} \dot{y}}{x} + \frac{2 \ddot{y}}{x^2} = 0
\]

Again, following a discussion similar to the one for solving equations in (38), \( 1 + \rho_i = \rho_{i+1} \). Thus, along each piece of \( \gamma^* \), the augmented Lagrangian \( L = \rho \frac{\zeta}{m} x \dot{y} + \zeta \frac{\dot{x}^2 + \dot{y}^2}{x} \) and \( \rho \) is a constant. We have shown that \( \gamma^* \) is an optimal solution of following calculus of variations problem:

\[
\text{Min}_{\gamma} J = \int_0^{t_f} \frac{\zeta}{m} \frac{x^2 + y^2}{x} dt
\]

subject to: \((x(0), y(0)) \) and \( \int_0^{t_f} \frac{\zeta}{m} \left( \frac{x^2}{x^2} - \frac{u^2}{x} y \right) dt \) are prescribed and \((x(t_f), y(t_f)) = (x(0), y(0)) \).

Based on (22), \( \frac{\dot{x}^2 + \dot{y}^2}{x} = u^2 + v^2 \). Apparently, problem (31) is equivalent to problem (32).

**Remark 2.** Sivak and Crooks [33] suggested that obtaining efficient performance of molecular machines requires minimization of dissipation. Theorem 3.1 gives a mathematical basis for why this must be so.

3.2. Maximum efficiency protocols of the heat engine. On the sub-Riemannian manifold \( N \) of the heat engine, for a trajectory \( \gamma : t \in [0, t_f] \to N \), \( \dot{\gamma} \in T_{\gamma(t)}N \) is its tangent vector field and \( p \in T^*_{\gamma(t)}N \) is a cotangent vector field, such that \( p \cdot \dot{\gamma} = 0 \). In canonical coordinates, \( p = (p_1, p_2, p_3)^T \) and we let \( \langle p, \dot{\gamma} \rangle_d = p^T \dot{\gamma} \). The pair \( \lambda = (p, \gamma) \in T^*N \), where \( T^*N \) is the cotangent bundle of \( N \). (Here \( \lambda \) is not to be confused with the \( \lambda \) notation for system parameter.) Here, we would like to consider optimal solutions to problem (32) with non-zero controls. In other words, these optimal solutions are regular extremals. In the case of the stochastic oscillator, \( f_1 = (\sqrt{\frac{3}{2} \zeta}, 0, \frac{\dot{z}^{3/2}}{m} \frac{y^2}{x^{5/2}})^T \) and \( f_2 = (0, \sqrt{\frac{3}{2} \zeta}, -\frac{\dot{z}^{3/2}}{m} \frac{y^2}{x^{5/2}})^T \) denote vector fields of the control system (22). From the Pontryagin maximum principle [1] [2], at time \( t \in [0, t_f] \), the sub-Riemannian Hamiltonian is the smooth function of \( T^*N \) defined as follows

\[
H : T^*N \to \mathbb{R}, \quad H(\lambda) = \max_{u,v} \left( \langle p, uf_1 + vf_2 \rangle_d - \frac{u^2 + v^2}{2} \right).
\]

So, in the case of the stochastic oscillator, the optimal control in canonical coordinates is given by

\[
u^* = \langle p, f_1 \rangle_d = \sqrt{\frac{3}{2} \zeta} p_1 + \frac{\dot{z}^{3/2}}{m} \frac{y^2}{x^{5/2}} p_3 \]

\[
u^* = \langle p, f_2 \rangle_d = \sqrt{\frac{3}{2} \zeta} p_2 - \frac{\dot{z}^{3/2}}{m} \frac{y}{x} p_3.
\]
Correspondingly,

\[ H(p, \gamma) = \frac{1}{2} \left( (p^T f_1)^2 + (p^T f_2)^2 \right) = \frac{1}{2} \left( (u^*)^2 + (v^*)^2 \right). \]  

(43)

In particular, every regular extremal trajectory is smooth and it is a solution of the Hamiltonian system \( \dot{\lambda} = \vec{H}(\lambda) \), where \( \vec{H} \) is the Hamiltonian vector field. Here \( \{ , \} \) is the canonical Poisson bracket. In canonical coordinates, for a real-valued function \( f \) of \( \lambda \),

\[ \vec{H}(f) = \{ f, H \} = \left( \frac{\partial H}{\partial p} \right)^\top \frac{\partial f}{\partial \gamma} - \left( \frac{\partial H}{\partial \gamma} \right)^\top \frac{\partial f}{\partial p} \]  

(44)

If \( \lambda(0) \) is the initial condition, the solution of the Hamiltonian system is \( \hat{\lambda}(t) = e^{t \vec{H}}(\lambda(0)) \) and

\[ \dot{p} = \frac{\partial H}{\partial \gamma} = -u^* D_\gamma (p^T f_1) - v^* D_\gamma (p^T f_2) \]

\[ \dot{\gamma} = \frac{\partial H}{\partial p} = (p^T f_1) f_1 + (p^T f_2) f_2 = u^* f_1 + v^* f_2 \]  

(45)

where \( p_3 \) is observed to be a conserved quantity. As \( \vec{H} = \{ H, H \} = 0 \), \( H \) is also a constant along the trajectory of \( \vec{H} \). \( (u^*, v^*) \) can be parameterized as \( (\sqrt{2H} \cos \phi, \sqrt{2H} \sin \phi) \) and

\[ u^* = \{ u^*, H \} = v^* \{ u^*, v^* \} \]

\[ v^* = \{ v^*, H \} = u^* \{ v^*, u^* \} \].  

(46)

Thus, in the case of the stochastic oscillator,

\[ \dot{\phi} = -\{ u^*, v^* \} = \frac{p_2}{2 \sqrt{\zeta}} - \frac{3 \zeta^{3/2} y}{2 m} x p_3 \]  

(47)

To replace \( p_2 \) in the equation for \( \dot{\phi} \), from \( v^* = \sqrt{2H} \sin \phi = \sqrt{x} p_2 - \frac{\zeta^{3/2} y}{\sqrt{2} m} x p_3 \), we get \( p_2 = \frac{\zeta y}{m x} p_3 + \sqrt{\frac{2H}{x}} \sin \phi \). The necessary condition for the heat engine (22) to work with maximum efficiency gives a trajectory on \( N \) with dynamics:

\[ \dot{x} = \sqrt{\frac{2H x}{\zeta}} \cos \phi; \quad \dot{y} = \sqrt{\frac{2H x}{\zeta}} \sin \phi \]

\[ \dot{\phi} = \frac{1}{2} \sqrt{\frac{2H}{x}} \sin \phi - \frac{\zeta^{3/2} y}{m x} p_3. \]  

(48)

**Definition 3.2.** In general, along a regular extremal trajectory of \( \vec{H} \), starting from \( \gamma(0) \in N \), at time \( t \) we define the \( t \)-exponential map of the optimal solution:

\[ \mathcal{E}_{\gamma(0)} : \mathbb{R}^+ \times T^*_\gamma(0) N \to N, \quad \mathcal{E}_{\gamma(0)}(t, \hat{\lambda}(0)) = \pi \left( e^{t \vec{H}}(\hat{\lambda}(0)) \right) \]  

(49)

where \( \pi \) is a projection from \( T^* N \) to \( N \).

In the case of the stochastic oscillator, as \( \gamma(0) \) is fixed, the information pertinent to \( \hat{\lambda}(0) \) is determined by \( \phi(0), H \) and \( p_3 \). We can write \( \hat{\lambda}(0) = \hat{\lambda}(\phi(0), H, p_3) \).

Also, along a regular extremal in the time interval \( [0, t_f] \), \( \forall t \in [0, t_f] \), if \( \gamma^*(t) \) belongs to a bounded region and \( \dot{\gamma}^*(t) \) is piece-wise continuous and satisfies a Lipschitz condition in that region, there exists a unique solution \( \gamma^*(t) \) to the Cauchy
problem: \[ \dot{\gamma}^* = u^* f_1 + v^* f_2, \gamma^*(0) \text{ is fixed.} \] (50)

The t-exponential map of a heat engine can also be written as
\[ F : \mathbb{R}^+ \times L^2_{[0,t_f]} \times L^2_{[0,t_f]} \to N, \; F(t,u^*,v^*) = \gamma^*(0) + \int_0^t (u^* f_1 + v^* f_2) \, dt'. \] (51)

At time \( t \), the partial differential of the t-exponential map at \((u^*, v^*)\) is the map:
\[ D_{(u^*,v^*)} F : L^2_{[0,t_f]} \times L^2_{[0,t_f]} \to T_{\gamma(t)} N, \; D_{(u^*,v^*)} F(u_p,v_p) = \int_0^t P_{\tau}^t (u_p f_1 + v_p f_2) \, dt' \] (52)

where \( P_{\tau}^t : \gamma^*_\tau(\tau) \to \gamma^*(t) \) is the flow generated by \((u^*, v^*)\), \( P_{\tau}^t \) is its push-forward operator [2] and \((u_p, v_p)\) is the perturbation in control.

3.3. Conjugate point theory and working cycles. In the last subsection, we saw that protocol (working loop) for a heat engine of maximum efficiency, under the condition of being a regular extremal, satisfies the Hamilton equations associated to the Pontryagin maximum principle. Among these extremal working loops, there is a special class called \textit{working cycles}. By analyzing the working cycles via conjugate point theory, the optimality of working loops is investigated.

**Definition 3.3.** For a heat engine operating along extremal working loops, from time 0 to time \( t_f \), we say the protocol is a working cycle if it satisfies the following conditions:

1. \[ x(0) = x(t_f), \; y(0) = y(t_f); \]
2. \[ \phi(0) = 2\pi \text{ and } \phi \text{ is monotonically decreasing.} \]

Along a loop in the space of \((x, y)\), by Stokes’ theorem, one writes a line integral as a surface integral:
\[ \psi(t_f) = \int \frac{\zeta^2}{m} \frac{y^2}{x^2} \, dx - \frac{\zeta^2}{m} \frac{y}{x} \, dy = \iint -\frac{\zeta^2}{m} \frac{y}{x^2} \, dx \, dy. \] (53)

Condition 1 and 2 are sufficient conditions to have the working cycle be a periodic and clock-wise trajectory in the space of \((x, y)\), by which we can extract positive mechanical work from the heat bath. Moreover, the time \( t_f \) is the period of the working cycle.

As in the case for geodesics in Riemannian geometry, along a geodesic on a sub-Riemannian manifold, at time \( t \), the image of t-exponential map may turn out to be a conjugate point, beyond where the geodesic will lose optimality. The conjugate point theory of sub-Riemannian geometry is well-developed in [2], and we apply this to our heat engine problem.

**Definition 3.4.** In general, fix \( \gamma(0) \in N \) and consider the t-exponential map \( E_{\gamma(0)}(t, \lambda(0)) \). A point \( \gamma(t) \neq \gamma(0) \) is said conjugate to \( \gamma(0) \), if \( \gamma(t) \) is a critical value for \( E_{\gamma(0)}(t, \lambda(0)) \) at time \( t \).

Following the definition of a working cycle, we will prove that at time \( t_f \), \( \gamma(t_f) \) is a conjugate point to \( \gamma(0) \).

**Theorem 3.5.** Along a regular extremal of our heat engine which satisfies conditions 1 and 2 in the definition of a working cycle, \( \gamma(t_f) \neq \gamma(0) \) and it is conjugate to \( \gamma(0) \).
Proof. Along a working cycle of the stochastic oscillator, as $x$ and $y$ are positive, $\psi(t_f) = \int \frac{\xi^2 x^2}{m} dx - \int \frac{\xi^2 y^2}{m} dy = \int \frac{\xi^2}{m} y^2 dxdy > 0$. $\gamma(t_f) \neq \gamma(0)$.

Once we choose the initial condition $\gamma(0)$ for a working cycle, its t-exponential map $E_{\gamma(0)}(t, \lambda(0))$ is a function of time $t$ and $\lambda(0) = \lambda(\phi(0), p_3)$. We take $H = \frac{1}{2}$.

To show $\gamma(t_f) = E_{\gamma(0)}(t, \tilde{\lambda}(0))$ is conjugate to $\gamma(0)$, it is necessary to show that the differential of the t-exponential map is not surjective. To prove that the differential is not surjective, it is enough to prove that
\[ \frac{\partial}{\partial \phi(0)} |_{t=t_f} E_{\gamma(0)}(t, \tilde{\lambda}(0)) = 0. \] (54)

At time $t_f$, as a working cycle is an optimal working loop, for the stochastic oscillator: $x(0) = x(t_f)$, $y(0) = y(t_f)$. Thus, along a regular extremal of a heat engine model,
\[ \frac{\partial x(t_f)}{\partial \phi(0)} = \frac{\partial y(t_f)}{\partial \phi(0)} = 0. \] (55)

As $\phi$ is monotonically decreasing ($\dot{\phi} < 0$), $x$ and $y$ can be re-parameterized by $\phi$. Thus,
\[ \psi(t_f) = \int_0^{t_f} \frac{\xi^2}{m} \left( \frac{y^2}{x^2} \dot{x} - \frac{y}{x} \dot{y} \right) dt = \int_{\phi(0)}^{\phi(t_f) - 2\pi} \frac{\xi^2}{m} \left( \frac{y^2}{x^2} \frac{dx}{d\phi} - \frac{y}{x} \frac{dy}{d\phi} \right) d\phi. \] (56)

By direct calculation, as a working cycle is a periodic trajectory of (48) in the space of $(x, y)$, it follows that $\frac{\partial \phi(t_f)}{\partial \phi(0)} = 0$ and $\frac{\partial}{\partial \phi(0)} E(t_f, \tilde{\lambda}(0))$ is a zero-vector. Therefore, rank of the differential of the t-exponential map is less than 3 and a working cycle will give us a conjugate point to $\gamma(0)$ at time $t_f$.

Moreover, the appearance of conjugate point will destroy optimality of a regular extremal. On that, without proof we state a theorem below. For more details, refer to [2]. See also [26].

**Theorem 3.6.** Let $\gamma^*$ be a working cycle. $\gamma^*(t)$ is not conjugate to $\gamma^*(0)$ for every $0 \leq t < t_f$. The extremal $\gamma$ is a strong minimum and the period time $t_f$ of the working cycle is called conjugate time of this extremal.

**Remark 3.** For an extremal working loop of a heat engine, whose monotonically decreasing phase angle $\phi$ does not reach $\phi(0) - 2\pi$, it is a strong minimum over the time interval $[0, t_f]$.

4. **Numerical design of working loops.** In the last section, for the stochastic oscillator, we showed the necessary condition for a maximum efficiency working loop. Also, based on the conjugate point analysis, a sufficient condition for the optimality of the maximum efficiency working loops is given. As a cyclically operated machine, the working loops of a heat engine are of special interest to design. The time span of a working loop is a key quantity in the design. To have this important information, firstly, we apply level set methods to solve the reachability problem of the engine. By fixing the initial condition of a protocol, we can obtain the time spans and ending points of working loops which start from the same point in the parameter space with initially zero extracted mechanical work.
Secondly, with the end-points and time span of the working loops, we reconstruct these working loops by mid-point approximation. To reduce the resulting numerical errors between the starting points and ending points in the space of the system parameter along each reconstructed trajectory, we refine the trajectories using shooting method. After carrying out the preceding three steps, we obtain maximum-efficiency working loops of the heat engine. The efficiencies of the engine working along different working loops are calculated and compared (see Table 2).

4.1. Level set methods. Over a time interval \([0, t]\), the working loops of the stochastic oscillator satisfy the condition \(x(0) = x(t)\) and \(y(0) = y(t)\).

As the heat engine is controllable (see section 2.3), starting from a point \(q^0 = (x^0, y^0, \psi = 0)\), over the time interval \([0, t]\), the ending points of all minimum path dissipation protocols in the space of \((x, y, \psi)\) of the engine form a set

\[
\{\gamma^*(t)|\gamma^*: \mathbb{R} \rightarrow N \text{ is a regular extremal and } \gamma^*(0) = q^0\}
\]  

(57)

This set is the reachable set of the heat engine at time \(t\). \(\forall t \in [0, t_{max}]\), with fixed \(q^0\), the union of reachable sets

\[
R(q^0)_{t \leq t_{max}} = \cup_{t \leq t_{max}} \{\gamma^*(t)|\gamma^*: \mathbb{R} \rightarrow N \text{ is a regular extremal and } \gamma^*(0) = q^0\}
\]  

(58)

is the set of all reachable points till time \(t_{max}\).

In this set \(R(q^0)\), we can select the points which satisfy the working loop condition. Thus, given a heat engine model, the first step to design working loops is to compute the collection of reachable sets till \(t_{max}\). For design purpose, \(t_{max}\) is sufficiently large. The reachable sets of some control problems can be computed by level set methods [28] [24]. See also [14] for recent developments. In the Appendix B, we will show that our control problem is numerically solvable by level set methods through the Hamilton-Jacobi equation:

\[
\frac{\partial \tilde{V}}{\partial t} + \sqrt{\frac{\partial \tilde{V}}{\partial q} \begin{pmatrix} \sqrt{x} \\ 0 \end{pmatrix}}_d^2 = 0. \tag{59}
\]

Following the discussion in Appendix C on rescaling the parameters \((x, y, \psi)\) of the stochastic oscillator to be \((\tilde{x}, \tilde{y}, \tilde{\psi})\), the Hamilton-Jacobi equation (59), with the new \(\tilde{V}\), turns out to be

\[
\frac{\partial \tilde{V}}{\partial t} + \sqrt{\frac{\partial \tilde{V}}{\partial q} \begin{pmatrix} \sqrt{x} \\ 0 \end{pmatrix}}_d^2 = 0. \tag{60}
\]

Rescaling \((x, y, \psi)\) to \((\tilde{x}, \tilde{y}, \tilde{\psi})\) is for the ease of implementing the level set methods by having the range of the \(\tilde{x}, \tilde{y}\) and \(\tilde{\psi}\) in the same scale. Having the \((\tilde{x}(0), \tilde{y}(0), \tilde{\psi}(0)) = (4, 4, 0)\) with associated units, up to arc-length of 1, the reachable set of the stochastic oscillator in 3D is given by figure 2.

The reachable set provides the information about the distance between reachable points with \((\tilde{x}, \tilde{y}) = (4, 4)\) and positive \(\tilde{\psi}\) coordinates and the center of the reachable set \((\tilde{x}, \tilde{y}, \tilde{\psi}) = (4, 4, 0)\). We display the distance information in table 1. Due to the discretization of \(\psi\), the coordinate of \(\tilde{\psi}\) is of step size 0.0784.
Figure 2. Reachable set of a stochastic oscillator in 3D

Table 1. Information from the reachable set of the stochastic oscillator

| Point number | distance | $\tilde{\psi} - coordinate$ |
|--------------|----------|-----------------------------|
| 1            | 1.1126   | 0.1207                      |
| 2            | 1.5302   | 0.1991                      |
| 3            | 1.8331   | 0.2775                      |
| 4            | 2.0515   | 0.356                       |
| 5            | 2.2134   | 0.4344                      |
| 6            | 2.3471   | 0.5128                      |
| 7            | 2.4982   | 0.5913                      |
| 8            | 2.6546   | 0.6697                      |
| 9            | 2.8082   | 0.7481                      |
| 10           | 2.9525   | 0.8266                      |

4.2. Trajectory reconstruction. For the stochastic oscillator, from last section, the necessary condition for a unit-speed regular extremal in the space of $(\tilde{x}, \tilde{y}, \tilde{\psi})$ is given by

$$\dot{x} = \sqrt{x} \cos \phi, \quad \dot{y} = \sqrt{x} \sin \phi,$$

$$\dot{\phi} = \frac{1}{2\sqrt{x}} \cos \phi - \frac{\dot{y}}{\dot{x}} p_3$$  \hspace{1cm} (61)$$

where $p_3$ is a constant. The complete information $(\tilde{x}(t), \tilde{y}(t), \tilde{\psi}(t))$ of a regular extremal can be recovered from above reduced dynamics by quadrature. Given the time span $t_f$ of the extremal and the number of steps $N$ (we use $N = 75$ here) in the mid-point approximation, the step size $h = \frac{t_f}{N}$ and the reduced dynamics (61)
is approximated as

\[
\begin{align*}
\frac{\ddot{x}^{i+1} - \ddot{x}^i}{h} &= \sqrt{\frac{\dddot{x}^{i+1} + \dddot{x}^i}{2}} \cos \left( \frac{\phi^{i+1} + \phi^i}{2} \right), \\
\frac{\ddot{y}^{i+1} - \ddot{y}^i}{h} &= \sqrt{\frac{\dddot{x}^{i+1} + \dddot{x}^i}{2}} \sin \left( \frac{\phi^{i+1} + \phi^i}{2} \right), \\
\frac{\phi^{i+1} - \phi^i}{h} &= \frac{1}{\sqrt{2(\dddot{x}^{i+1} + \dddot{x}^i)}} \cos \left( \frac{\phi^{i+1} + \phi^i}{2} \right) - \left( \frac{\dddot{y}^{i+1} + \dddot{y}^i}{\dddot{x}^{i+1} + \dddot{x}^i} \right) p_3
\end{align*}
\]

(62)

where \( \dddot{x}^i, \dddot{y}^i, \phi^i \) are the values of \( \dddot{x}, \dddot{y}, \phi \) at time \( ih \) (\( i = 0, 1, \ldots, N \)). There are \( x^0, \ldots, x^N, y^0, \ldots, y^N, \phi^0, \ldots, \phi^N \) and \( p_3 \), in total \( 3N + 4 \) variables. Based on the definition of a working loop

\[
\dddot{x}^0 = \dddot{y}^N = 4, \quad \dddot{y}^0 = \dddot{y}^N = 4.
\]

(63)

There are \( 3N \) unknowns, \( X = (\dddot{x}^0, \ldots, \dddot{x}^{N-1}, \dddot{y}^0, \ldots, \dddot{y}^{N-1}, \phi^0, \ldots, \phi^N, p_3)^T \) in the \( 3N \) equations (62). The problem can be solved by Newton-Raphson method. In the solution, we pick up the values of \( \phi(0) \) and \( p_3 \) and bring them to (61) with \( (\dddot{x}(0), \dddot{y}(0)) = (4, 4) \). Thus, the ordinary differential equation (61) from time 0 to time \( t_f \) can be numerically solved. Using shooting method, by varying the initial value of \( \phi \) around the solution from mid-point approximation, the differences between \( (\dddot{x}(0), \dddot{y}(0)) \) and \( (\dddot{x}(t_f), \dddot{y}(t_f)) \) which are measured by Euclidean distances are minimized to have the numerical solution to be close to a working loop. Figure 3 is the projection of the reconstruction trajectory with dissipation of 1.1126 into \( (\dddot{x}, \dddot{y}) \) space. The Euclidean distance between \( \dddot{x}(0) \) and \( \dddot{x}(t_f) \) is 0.0058 and the Euclidean distance between \( \dddot{y}(0) \) and \( \dddot{y}(t_f) \) is 0.0026.

![Figure 3. Reconstruction of a working loop](image)
4.3. **Efficiencies of the heat engine.** By the definition of $\eta$ in (30),

$$\eta = \frac{\int_{0}^{t_f} \left( \frac{q^2}{m} \dot{x} - \frac{\dot{y}}{m} \right) dt}{\int_{0}^{t_f} \left( \frac{q^2}{m} \dot{x}^2 + \frac{q \dot{y}}{m} \right) dt + \frac{m}{\zeta} \left( \frac{q^2 t_f}{2} \right)}.$$  (64)

For a heat engine, the total heat supply is the sum of the heat supply from the heat engine and the dissipation along the working loop. Along the maximum efficiency working loop, the dissipation along the loop is the product of the length of the loop and the speed of the protocol $\nu$ as in (87). Along a maximum efficiency working loop of a stochastic oscillator

$$\eta = \frac{\int_{0}^{t_f} \left( \frac{q^2}{m} \dot{x} - \frac{\dot{y}}{m} \right) dt}{\int_{0}^{t_f} \left( \frac{q^2}{m} \dot{x}^2 + \frac{q \dot{y}}{m} \right) dt}.$$  (65)

If the corresponding unit-speed optimal control is $(\tilde{u}_0^*, \tilde{v}_0^*)$ with duration $t_{f,0}$, any other optimal control can be expressed as $(\nu \tilde{u}_0^*, \nu \tilde{v}_0^*)$ with duration $\nu^{-1} t_{f,0}$ and

$$\eta = \frac{\int_{0}^{\nu^{-1} t_{f,0}} \left( \frac{q^2}{m} \dot{x} - \frac{\dot{y}}{m} \right) dt}{\int_{0}^{\nu^{-1} t_{f,0}} \left( \frac{q^2}{m} \dot{x}^2 + \frac{q \dot{y}}{m} \right) dt}.$$  (66)

To operate the system in unit speed, $\nu = 1$, in the example of the stochastic oscillator, $\frac{\zeta}{\nu} = 0.1$ sec,

$$\eta = \frac{\int_{0}^{t_{f,0}} \left( \frac{q^2}{m} \dot{x} - \frac{\dot{y}}{m} \right) dt}{\int_{0}^{t_{f,0}} \left( \frac{q^2}{m} \dot{x}^2 + \frac{q \dot{y}}{m} \right) dt + 0.1 t_{f,0}}.$$  (67)

where $t_{f,0}$, $\tilde{u}_0^*$ and $\tilde{v}_0^*$ are associated to the unit-speed maximum efficiency working loop. Thus, the efficiencies of the stochastic oscillator along different working loops are listed in Table 2.

**Remark 4.** By comparing the efficiencies of the stochastic oscillator along different loops, it is seen that, the more energy the system dissipates into the environment, the more mechanical work it can extract and the efficiency of the working loop is higher.

**Remark 5.** Based on the equation (66) for efficiency, in the near-equilibrium regime, it is shown that the extracted mechanical work and the heat supply along an optimal working loop is independent of the speed $\nu$ and the dissipation is proportional to it. Hence, the faster the heat engine is operated along a maximum efficiency working loop, the higher the mechanical power which is the ratio of the extracted mechanical work per loop to the time span of the working loop. Meanwhile, the efficiency of the engine will be lower.
Table 2. Efficiencies of the engine along the maximum efficiency working loops

| Point number | Extracted mechanical work | Heat supply | Dissipation | \( \eta \) |
|--------------|---------------------------|-------------|-------------|----------|
| 1            | 0.1207                    | 0.8319      | 1.1126      | 0.1280   |
| 2            | 0.1991                    | 1.2085      | 1.5302      | 0.1462   |
| 3            | 0.2775                    | 1.5055      | 1.8331      | 0.1643   |
| 4            | 0.3560                    | 1.7363      | 2.0515      | 0.1834   |
| 5            | 0.4344                    | 1.9179      | 2.2134      | 0.2031   |
| 6            | 0.5128                    | 2.0771      | 2.3471      | 0.2218   |
| 7            | 0.5913                    | 2.2568      | 2.4982      | 0.2359   |
| 8            | 0.6697                    | 2.4464      | 2.6546      | 0.2470   |
| 9            | 0.7481                    | 2.6362      | 2.8082      | 0.2565   |
| 10           | 0.8266                    | 2.8185      | 2.9525      | 0.2655   |

5. **Conclusions.** This paper shows how to design heat engines that operate in non-equilibrium statistical mechanical settings through a concrete application of the methods of geometric optimal control to a model problem – the linear oscillator in contact with a heat bath. Treating stiffness and bath temperature as adjustable system parameters, we have formulated an optimal control problem viewed naturally in a sub-Riemannian geometric setting. Using the maximum principle of optimal control theory, the Hamilton-Jacobi-Bellman equation, and its solution using level-set methods, we have constructed protocols of maximum efficiency subject to constraint on work generated in a cycle, summarized in Table 2. These finite time protocols have efficiency below 1/3 and the efficiency increases monotonically with protocols of longer duration. The problem considered in this paper is an example of an underdamped system (with second order dynamics). In a forthcoming paper we tackle the overdamped limit case as illustrated by the Nyquist-Johnson resistor coupled to a controllable capacitor and a controllable heat bath. Additional statistical mechanical tools will be found necessary in such a case to achieve sub-Riemannian geometric structures as in the present work.

**Acknowledgments.** We are grateful for conversations on the subject of this paper with our colleagues Gavin Crooks, Christopher Jarzynski and Michael DeWeese. We have learned much from their papers. This work was supported by the ARL/ARO MURI Program Grant No. W911NF-13-1-0390, through the University of California Davis (as prime), the ARL/ARO Grant No. W911NF-17-1-0156, through the Virginia Polytechnic Institute and State University (as prime), and by Northrop Grumman Corporation.

A. **Linear response theory.** The key idea of linear response analysis in this article is to use a piecewise constant over time protocol to approximate the continuously time-varying one. Assuming our statistical mechanical system is at equilibrium at time \( t = 0 \), with control parameter \( \lambda_0 \), it is subject to a protocol \( \lambda(t) \), where \( \lambda(0) = \lambda_0 \). At time 0, the system is perturbed by \( \dot{\lambda}(0) \). This process is approximated as follows where linear response theory is applicable [37].

The statistical mechanical system reaches equilibrium from time \( -\infty \) to time \( t = 0 \) with control parameter \( \lambda_0 + (\lambda_0 - \lambda(t_1)) \) (later we denote \( \lambda_0 - \lambda(t_1) \) as \( \Delta \lambda \)). At time \( t = 0 \), \( \Delta \lambda \) vanishes and at time \( t_1 \) (\( t_1 > 0 \)), the system is under investigation
with the control parameter $\lambda_0$ as the reference value. For this approximation process to be meaningful, let $\lim_{t_1 \to 0} \frac{\lambda_0 - (\lambda_0 + (\lambda_0 - \lambda(t_1)))}{t_1} = \dot{\lambda}(0)$.

In the approximation process, from time $-\infty$ to time $t = 0$, the system arrives at an equilibrium distribution with control parameter $\lambda_0 + \Delta \lambda$. So, the equilibrium probability distribution at time $t = 0$ is $\rho_{eq,\lambda_0 + \Delta \lambda}(\xi) = \frac{e^{-\beta H(\xi,\lambda_0 + \Delta \lambda)}}{Z(\lambda_0 + \Delta \lambda)}$ and the equilibrium distribution with control parameter $\lambda_0$ is $\rho_{eq,\lambda_0}(\xi) = \frac{e^{-\beta H(\xi,\lambda_0)}}{Z(\lambda_0)}$. By the linearization of $\beta H$,

$$\frac{\rho_{eq,\lambda_0 + \Delta \lambda}(\xi)}{\rho_{eq,\lambda_0}(\xi)} = \frac{e^{-\beta H(\lambda_0 + \Delta \lambda,\xi) - \beta H(\lambda_0,\xi)}}{Z(\lambda_0 + \Delta \lambda)/Z(\lambda_0)} \approx (1 - X^T \Delta \lambda + O(\Delta \lambda^2))(1 + (X^T)_{eq,\lambda} \Delta \lambda + O(\Delta \lambda^2)).$$ (68)

Following static linear response theory,

$$\rho_{eq,\lambda_0 + \Delta \lambda} \approx \rho_{eq,\lambda_0} - \rho_{eq,\lambda_0} \Delta X^T \Delta \lambda. \quad (69)$$

At time $t_1$,

$$\langle \Delta X \rangle = \int \rho(\xi, t_1) \Delta X d\xi = \int \rho_{eq,\lambda_0 + \Delta \lambda}(\xi_0) \Delta X \rho(\xi, t_1|\xi_0, \lambda_0 + \Delta \lambda) d\xi d\xi_0. \quad (70)$$

Denote $\Delta X(t_1) = \int \Delta X d\rho(\xi, t_1|\xi_0, \lambda_0 + \Delta \lambda) d\xi$ and use the result in (69),

$$\langle \Delta X \rangle = \int \rho_{eq,\lambda_0 + \Delta \lambda}(\xi_0) \Delta X(t_1) d\xi_0 \approx - \langle \Delta X(t_1) \Delta X^T \rangle_{eq,\lambda_0} \cdot \Delta \lambda. \quad (71)$$

On the other hand, based on dynamic linear (step) response theory, at $t_1 > 0$, $\langle \Delta X \rangle \approx \int_{t_1}^{\infty} \chi(t_1 - t') (\lambda(t') - \lambda(t_1)) dt'$. From time $-\infty$ to time $0$, $\lambda(t') - \lambda(t_1) = \Delta \lambda$.

Do change of variable $s = t_1 - t'$ and $ds = -dt'$.

$$\langle \Delta X \rangle \approx \int_{t_1}^{\infty} \chi(s) ds \cdot \Delta \lambda$$ (72)

where $\chi$ is the linear response kernel. Comparing the results from both static linear response theory (71) and dynamic linear response theory (72), $\int_{t_1}^{\infty} \chi(s) ds = - \langle \Delta X(t_1) \Delta X^T \rangle_{eq,\lambda_0}$. Assuming that $\langle \Delta X(s) \Delta X^T \rangle$ is differentiable against $s$ and $\lim_{s \to \infty} \langle \Delta X(s) \Delta X^T \rangle = 0$,

$$\chi(s) = \frac{d}{ds} \langle \Delta X(s) \Delta X^T \rangle_{eq,\lambda_0}. \quad (73)$$

Looking into the integral $\langle \Delta X(s) \Delta X^T \rangle_{eq,\lambda_0}$ carefully,

$$\langle \Delta X(s) \Delta X^T \rangle_{eq,\lambda_0} = \int \left( \int \Delta X(\xi) \rho(\xi, s|\xi_0, 0) d\xi \right) \rho_{eq,\lambda_0}(\xi_0) \Delta X^T(\xi_0) d\xi_0. \quad (74)$$

As $\Delta \lambda \to 0$,

$$\langle \Delta X(s) \Delta X^T \rangle_{eq,\lambda_0} = \int \int \Delta X(\xi) \Delta X^T(\xi_0) \rho(\xi, s; \xi_0, 0) d\xi d\xi_0 \quad (75)$$

where $\rho(\xi, s; \xi_0, 0)$ is the joint probability density of $\xi$ and $\xi_0$.

Let us apply dynamic linear response theory to the real process with the approximated linear response kernel (73). Based on the assumption $\lim_{s \to \infty} \langle \Delta X(s) \Delta X^T \rangle = 0$,
use change of variable \( s = t_1 - t' \) and integration-by-parts in the integral of dynamic linear response,

\[
\langle \Delta X \rangle \approx \int_{-\infty}^{t_1} \chi(t_1 - t') \cdot (\lambda(t') - \lambda(t_1)) dt'
\]

\[
= \int_{0}^{\infty} \chi(s) \cdot (\lambda(t_1 - s) - \lambda(t_1)) ds
\]

\[
= \int_{0}^{\infty} \frac{d}{ds} \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} \cdot (\lambda(t_1 - s) - \lambda(t_1))
\]

\[
= \int_{0}^{\infty} \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} \cdot \dot{\lambda}(t_1 - s) ds.
\]

(76)

**Theorem A.1.** In our heat engine, there are two time scales: one is fast time scale of fluctuations in the statistical mechanical system and the other is slow time scale of the system parameter. The system parameter varies slowly to have the system operating near its corresponding equilibrium. In other words, we have following assumption:

1. \( \forall s \in [0, \infty), \| \dot{\lambda}(t_1 - s) - \dot{\lambda}(t_1) \|_{\infty} < A \), where \( A \) is a positive constant and \( \| \|_{\infty} \) stands for supremum norm.

2. At time \( s \), every element in the covariance matrix \( \langle \Delta X(s) \Delta X^\top \rangle \) is upper-bounded with an exponentially decaying term \( Be^{-s/\tau} \), where \( B \) and \( \tau \) are positive constants.

With these assumption, up to order \( O(\tau A) \), we have an inverse diffusion tensor to approximate the average dissipation rate \( d \).

Proof.

\[
\langle \Delta X \rangle - \int_{0}^{\infty} \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} ds \cdot \dot{\lambda}(t_1) = \int_{0}^{\infty} \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} \cdot \dot{\lambda}(t_1 - s) ds - \int_{0}^{\infty} \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} ds \cdot \dot{\lambda}(t_1) = \int_{0}^{\infty} \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} \cdot \left( \dot{\lambda}(t_1 - s) - \dot{\lambda}(t_1) \right) ds.
\]

(77)

Thus,

\[
\| \langle \Delta X \rangle - \int_{0}^{\infty} \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} ds \cdot \dot{\lambda}(t_1) \|_{\infty} \leq \int_{0}^{\infty} \| \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} \cdot \left( \dot{\lambda}(t_1 - s) - \dot{\lambda}(t_1) \right) \|_{\infty} ds.
\]

(78)

With a short calculation, if \( n \) is the dimension of \( \dot{\lambda} \),

\[
\int_{0}^{\infty} \| \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} \cdot \dot{\lambda}(t_1 - s) - \dot{\lambda}(t_1) \|_{\infty} ds < 2\tau nAB.
\]

(79)

Thus, up to order \( O(\tau A) \), at time \( t_1 \), \( \langle \Delta X \rangle \) is approximated by

\[
\int_{0}^{\infty} \langle \Delta X(s) \Delta X^\top \rangle_{eq,\lambda_0} ds \cdot \dot{\lambda}(t_1).
\]

(80)
Moreover, because of smoothness of $\lambda(t)$, \[ \lim_{t_1 \to 0} \dot{\lambda}(t_1) = \dot{\lambda}(0) \]

\[ \langle \Delta X \rangle \approx \hat{\Delta} \int_0^\infty \langle \Delta X(s) \Delta X^\top \rangle_{eq, \lambda_0} ds \cdot \dot{\lambda}(0) \]  

(81)

\[ d = \dot{\lambda}(0) \langle \Delta X \rangle \approx \left[ \frac{d\lambda^\top}{dt} \right]_{t=0} g[\lambda_0] \left[ \frac{d\lambda}{dt} \right]_{t=0} \]  

(82)

with the inverse diffusion tensor

\[ g_{ij} \equiv \hat{\Delta} \int_0^\infty \langle \Delta X_j(s) \Delta X_i \rangle_{eq, \lambda_0} ds. \]  

(83)

The detailed calculation of the inverse diffusion tensor of the stochastic oscillator is in [35].

B. Hamilton-Jacobi-Bellman equation. Given the heat engine,

\[ \dot{\gamma} = uf_1 + vf_2 \]  

(84)

where curve $\gamma : \mathbb{R} \to N$ and $N$ is the sub-Riemannian manifold of the heat engine. $(u, v)$ is the control and $(f_1, f_2)$ are vector fields. Over the time interval $[0, t_f]$, the dissipation of a protocol $\Lambda$ (scaled by a constant $\frac{1}{2}$)

\[ J(\gamma) = \frac{1}{2} \int_0^{t_f} (u^2 + v^2) dt. \]  

(85)

Compare with the associated arc-length of the curve $\gamma$ on the sub-Riemannian manifold $N$

\[ l(\gamma) = \int_0^{t_f} \sqrt{u^2 + v^2} dt. \]  

(86)

From [33], it is known that the dissipation $J$ is the geometric energy of the curve $\gamma$. As in Riemannian geometry, in [2], Lemma 3.47, it is proved that minimizing the arc-length of the curve is equivalent to minimizing the geometric energy of the curve.

Along a unit-speed minimizer $\gamma^* (u^2 + v^2 = 1)$, starting from point A to point B on the manifold $N_i$, over the time interval $[0, t_f]$, the length $l(\gamma^*) = t_f$. Traveling along the extremal trajectory at a different speed $\nu$ from A to B, the minimum length (i.e. the distance between two points on the sub-Riemannian manifold) is invariant but the dissipation along the extremal (i.e. the geometric energy)

\[ J = \frac{l^2}{2t_f} = \frac{t_f \nu^2}{2}. \]  

(87)

Thus, instead of directly computing reachable sets of a heat engine with minimum dissipation, we can compute reachable sets of the heat engine with the minimum arc-length. Based on the information from the reachable sets, we can compute the minimum dissipation by (87).

To minimize the arc-length for a heat engine, by Pontryagin’s maximum principle,

\[ H : T^* N \to \mathbb{R}, \quad H(\dot{\lambda}) = \max_{u,v} \left( \langle p, uf_1 + vf_2 \rangle_d - \sqrt{u^2 + v^2} \right), \]  

(88)
It follows that the optimal control is
\[ u^* = \langle p, f_1 \rangle_d \sqrt{u^{*2} + v^{*2}} \]  
\[ v^* = \langle p, f_2 \rangle_d \sqrt{u^{*2} + v^{*2}}. \]  
(89)

Bringing the \((u^*, v^*)\) into \(H\), the Hamiltonian is zero. Moreover, as it is shown in [2], the minimizers are of constant speed. In the case of unit-speed extremals \((\sqrt{u^{*2} + v^{*2}} = 1)\),
\[ H = \sqrt{\langle p, f_1 \rangle_d^2 + \langle p, f_2 \rangle_d^2} - 1 = 0 \]  
(90)
which gives us
\[ \sqrt{\langle p, f_1 \rangle_d^2 + \langle p, f_2 \rangle_d^2} = 1 \]  
(91)

On the other hand, by the approach of dynamic programming, to minimize the cost function,
\[ l(t, \gamma(t), u, v) = \int_t^{t_f} \sqrt{u^2 + v^2} \, dt \]  
(92)
where \(L(t, \gamma(t), u(t), v(t)) = \sqrt{u^2(t) + v^2(t)}\) is the Lagrangian and \(\gamma\) is a curve starting from a point in \(N\) and \(\gamma(t_f) = q_0\). We have the value function over the time interval \([0, t_f]\)
\[ \hat{V}(t, \gamma(t)) \equiv \inf_{(u,v)} l(t, \gamma(t), u(t), v(t)). \]  
(93)

A sufficient condition for optimality of the geodesics on the sub-Riemannian manifold is: there is a \(C^1\) function \(\hat{V}: [0, t_f] \times \mathbb{R}^n \to \mathbb{R}\) satisfying Hamilton-Jacobi-Bellman equation [22]
\[ -\frac{\partial \hat{V}}{\partial t}(t, \gamma(t)) = \inf_{(u,v)} \left\{ L(t, \gamma(t), u(t), v(t)) + \left\langle \frac{\partial \hat{V}}{\partial \gamma}(t, \gamma(t)), \dot{\gamma} \right\rangle \right\} \]  
(94)
\((\forall t \in [0, t_f] \text{ and } \forall \gamma(t) \in N)\) and the boundary condition
\[ \hat{V}(t_f, \gamma(t_f)) = 0. \]  
(95)

Supposing that there exists a control \((u^*, v^*)\) and the corresponding trajectory \(\gamma^*: [0, t_f] \to N\), with a given initial condition, satisfying the equation
\[ L(t, \gamma^*(t), u^*(t), v^*(t)) + \left\langle \frac{\partial \hat{V}}{\partial \gamma^*}|_{\gamma^*, \dot{\gamma}^*} \right\rangle_d \]  
\[ = \inf_{(u,v)} \left\{ L(t, \gamma_i(t), u(t), v(t)) + \left\langle \frac{\partial \hat{V}}{\partial \gamma}|_{\dot{\gamma}} \right\rangle \right\}, \]  
(96)
then compare (96) with Pontryagin maximum principle,
\[ H \left( t, \gamma^*, u^*, v^*, -\frac{\partial \hat{V}}{\partial \gamma}|_{\gamma^*} \right) = \max_{u,v} \left( \langle p, uf_1 + vf_2 \rangle_d - \sqrt{u^2 + v^2} \right). \]  
(97)

It is then seen that along a regular extremal
\[ p = -\frac{\partial \hat{V}}{\partial \gamma}|_{\gamma^*}. \]  
(98)

In the space of \((x, y, \psi)\), based on [29], there exists a function \(\hat{V}: (t, q) \to \mathbb{R}\), which is monotonically decreasing with time, where \(q \in N\) and \(\hat{V}(t(q), q) = 0\) is equivalent
to the fact that there \( \exists !' \) and \( \hat{V}(t', \gamma^*(t') = q) = \hat{t}(q) \) (i.e. the distance between the \( q \) and \( q' \) is \( \hat{t}(q) \)). Thus, on the level surface \( \hat{V}(t(q), q) = 0 \)

\[
\frac{d\hat{V}}{dq} = \frac{\partial \hat{V}}{\partial q} + \frac{\partial \hat{V}}{\partial t} \frac{\partial t}{\partial q} = 0. \tag{99}
\]

Given that \( \frac{\partial \hat{V}}{\partial t} < 0 \) \[29\],

\[
\frac{\partial \hat{V}}{\partial \gamma}\bigg|_{\gamma(t') = q} = \frac{\partial t}{\partial q} = -\frac{\partial \hat{V}}{\partial q} \frac{\partial t}{\partial \hat{V}} \tag{100}
\]

along the extremal \( \gamma^* \), \( \hat{p}(t') = -\frac{\partial \hat{V}}{\partial \gamma}\bigg|_{\gamma(t') = q} = \frac{\partial \hat{V}}{\partial q} \frac{\partial t}{\partial \hat{V}} \).

Bringing this expression of \( \hat{p} \) into (91)

\[
\sqrt{\left\langle \frac{\partial \hat{V}}{\partial q} \frac{\partial t}{\partial \hat{V}}, f_1 \right\rangle_d^2 + \left\langle \frac{\partial \hat{V}}{\partial q} \frac{\partial t}{\partial \hat{V}}, f_2 \right\rangle_d^2} = 1. \tag{101}
\]

We have a Hamilton-Jacobi equation,

\[
\frac{\partial \hat{V}}{\partial t} + \sqrt{\left\langle \frac{\partial \hat{V}}{\partial q} \frac{\partial t}{\partial \hat{V}}, f_1 \right\rangle_d^2 + \left\langle \frac{\partial \hat{V}}{\partial q} \frac{\partial t}{\partial \hat{V}}, f_2 \right\rangle_d^2} = 0. \tag{102}
\]

C. Rescaling in stochastic oscillator. In the stochastic oscillator, choosing \( k_0 \) as the initial value of \( k \), then as a deterministic oscillator, its natural frequency \( \omega_0 = \sqrt{\frac{k_0}{m}} \). To have this deterministic oscillator to be critically damped, \( \zeta = 2\sqrt{m/k_0} \) and \( \beta_0 \) is the initial value of the inverse temperature. In the space \( (x, y) \), the initial value is

\[
x_0 = \frac{1}{4\beta_0 k_0} \tag{103}
\]

\[
y_0 = \frac{1}{\beta_0 \zeta} \sqrt{\frac{m}{k_0}} = \frac{1}{2\beta_0 k_0} \sqrt{\frac{m}{k_0}} = \frac{1}{4\beta_0 k_0} = x_0 \tag{104}
\]

It indicates that \( x \) and \( y \) are of the same scale and of the same unit meter\(^2\). Choosing \( k_0 = 0.25 \times 10^{-7} \text{N/meter} = 0.25 \times 10^{-7} \text{kg/sec}^2 \), \( m = 1 \text{ng} = 10^{-12} \text{kg} \) and \( \beta_0 = \frac{1}{k_B T_0} = 2.473 \times 10^{20} \text{sec}^2/(\text{meter}^2 \text{kg}) \) \( (k_B = 1.38 \times 10^{-23} \text{meter(\sec)^{-1}})^2 \text{kg/K} \) and \( T_0 = 293 \text{K} \),

\[
x_0 = y_0 = 4.0436 \times 10^{-14} \text{meter}^2. \tag{105}
\]

Rescaling \( x \) and \( y \) by \( 10^{-14} \), we have

\[
x = \hat{x} \times 10^{-14}, \quad y = \hat{y} \times 10^{-14} \tag{106}
\]

\[
x = \hat{x} \times 10^{-14}, \quad \hat{x} = \hat{x} \times 10^{-14}, \quad \hat{y} = \hat{y} \times 10^{-14}. \tag{107}
\]

The average dissipation rate in the unit of \( k_B T/\text{sec} \) is

\[
\hat{d} = \zeta \left( \frac{\hat{x}^2 + \hat{y}^2}{x} \right) = \zeta \left( \frac{\hat{x}^2 \times 10^{-28} + \hat{y}^2 \times 10^{-28}}{\hat{x} \times 10^{-14}} \right) = \zeta \left( \frac{\hat{x}^2 + \hat{y}^2}{\hat{x}} \right) \times 10^{-14} \tag{108}
\]

and the extracted power is

\[
\hat{\psi} = \frac{C^2}{m} \left( \frac{\hat{y}^2 \hat{x} - \hat{y} \hat{y}}{\hat{x}^2} \right) = \frac{C^2}{m} \left( \frac{\hat{y}^2 \hat{x} - \hat{y} \hat{y}}{\hat{x}^2} \right) \times 10^{-14}. \tag{109}
\]
In consequence, the efficiency $\eta$ over a time interval $[0,t_f]$ is

$$\eta = \frac{\int_0^{t_f} \psi \, dt}{\int_0^{t_f} \left(\left(\frac{\dot{x}}{m} \frac{\ddot{y}}{y}\right) \mathbb{1}\{\frac{\dot{y}}{y} > 0\} + \tilde{d}\right) \, dt}$$

$$= \frac{\int_0^{t_f} \frac{\dot{x}^2}{m} \left(\frac{\ddot{y}}{y} \right) \times 10^{-14} \, dt}{\int_0^{t_f} \left(\frac{\dot{x}^2}{m} \frac{\ddot{y}}{y} \right) \times 10^{-14} \mathbb{1}\{\frac{\dot{y}}{y} > 0\} + \zeta \left(\frac{\dot{x}^2 + \dot{y}^2}{x}\right) \times 10^{-14} \, dt}$$

$$= \frac{\int_0^{t_f} \left(\frac{\dot{x}^2}{m} \frac{\ddot{y}}{y} \right) \mathbb{1}\{\frac{\dot{y}}{y} > 0\} + \left(\frac{\dot{x}^2 + \dot{y}^2}{x}\right) \mathbb{1}\{\frac{\dot{y}}{y} > 0\} \, dt}{\int_0^{t_f} \left(\frac{\dot{x}^2}{m} \frac{\ddot{y}}{y} \right) \mathbb{1}\{\frac{\dot{y}}{y} > 0\} + \left(\frac{\dot{x}^2 + \dot{y}^2}{x}\right) \mathbb{1}\{\frac{\dot{y}}{y} > 0\} \, dt}.$$  \tag{108}

Having $\zeta$ as a constant weighting factor between the extracted mechanical work and the dissipation, the scaled extracted mechanical power $\tilde{\psi} = \frac{\dot{y}^2}{y} \dot{x} - \frac{\dot{x}^2}{x} \dot{y}$ and $\tilde{\psi}(0) = 0$, it is straightforward to show that to find a maximum efficiency working loop of the stochastic oscillator is equivalent to the problem of finding an optimal protocol which minimizes

$$J = \int_0^{t_f} \frac{\dot{x}^2 + \dot{y}^2}{x} \, dt$$  \tag{109}

while $\int_0^{t_f} \left(\frac{\dot{x}^2}{m} \frac{\ddot{y}}{y} \right) \mathbb{1}\{\frac{\dot{y}}{y} > 0\} \, dt$ is a prescribed value and $(\dot{x}(0), \dot{y}(0)) = (\dot{x}(t_f), \dot{y}(t_f))$. The associated sub-Riemannian structure is given by

$$\begin{bmatrix} \frac{\dot{x}}{\sqrt{x}} \\ \frac{\dot{y}}{\sqrt{y}} \\ \frac{\dot{\psi}}{\sqrt{\psi}} \end{bmatrix} = \tilde{u} \begin{bmatrix} \frac{\sqrt{x}}{x} \\ 0 \\ \frac{\sqrt{\psi}}{\psi} \end{bmatrix} + \tilde{v} \begin{bmatrix} 0 \\ \frac{\sqrt{x}}{x} \\ \frac{\sqrt{\psi}}{\psi} \end{bmatrix}.$$  \tag{110}

where $(\tilde{u}, \tilde{v})$ is the new control and the new average dissipation rate is $\tilde{u}^2 + \tilde{v}^2$. The weighting factor in our example $\zeta = \frac{2\sqrt{m\kappa}}{m} = 10\text{sec}^{-1}.$

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Received February 2018; revised September 2018.

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