Ito-Langevin Model and Stochastic Thermodynamics Overview

Graphene-based Energy Harvesting
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Langevin Equation of Brownian Particle

- $\mathcal{H}(x, p, q) = \frac{p^2}{2m} + U(x) + \frac{q^2}{2C(x)} - \frac{C_0(V)V^2}{2d}x + qV$
- From Hamilton's Equations:

$$dx = v\,dt$$

$$mdv = \left[-\eta v - U'(x) - \frac{q^2 - C_0 V^2}{2C_0 V d}\right] dt + \sqrt{2T\eta}\, dw_p$$

Langevin Equation for Charge through Equivalent Resistor

- Some relations used later on:

$$\frac{\partial \mathcal{H}}{\partial q} = V + \frac{q}{C(x)}$$

- Langevin Equation:

$$dq = \left[\frac{\partial}{\partial q}\left(\frac{T}{\mathcal{R}}\right) - \frac{1}{\mathcal{R}}\frac{\partial \mathcal{H}}{\partial q}\right] dt + \sqrt{\frac{2T}{\mathcal{R}}}\, dw_q$$

Fokker-Planck Equation

- In general:

$$\frac{\partial \rho}{\partial t} = \sum_{i,j} \frac{\partial}{\partial A_i} \left(-k_B T [A_i, A_j] + \lambda_{ij} \frac{\partial \mathcal{H}}{\partial A_j} + \lambda_{ij} \frac{\partial}{\partial A_j} \right) \rho(\mathbf{A}, t)$$

- Our case:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x} \left(\frac{\partial \mathcal{H}}{\partial p} \rho \right) + \frac{\partial}{\partial p} \left[\frac{\partial \mathcal{H}}{\partial x} \rho + \eta \left(\frac{p}{m} \rho + T \frac{\partial \rho}{\partial p} \right) \right] +$$

$$\frac{\partial}{\partial q} \left[\frac{1}{\mathcal{R}} \left(\frac{\partial \mathcal{H}}{\partial q} \rho + T \frac{\partial \rho}{\partial q} \right) \right]$$

Solution to FPE

- constant Equivalent Resitance $\mathcal{R}$
- Stationary Solution is the Equilibrium Probability Density when

$$\frac{\partial \rho}{\partial t} = 0$$

$$\rho_0(\mathbf{A}) = const \times e^{\dfrac{-\mathcal{H}}{T}}$$

Average Generated Power

- POV of Grahpene Ripple

$$d'Q = \left(-\eta\frac{p}{m} + \sqrt{2T\eta}\frac{\mathrm{d}w_p}{\mathrm{d}t}\right) \circ dx(t)$$

$$= d\mathcal{H}(x,p,q) - \frac{\partial \mathcal{H}}{\partial q} \circ dq(t)$$

- Converting to an Ito Product:

$$d'Q = \frac{\eta}{m^2}(mT - p^2)dt + \sqrt{2T\eta}\frac{p}{m}dw_p(t)$$

Averages

- Average Heat Flux vanishes in equilibrium beacuse of equipartition theorem

$$\left\langle \frac{\mathrm{d}' Q}{\mathrm{d}t} \right\rangle = \frac{\eta}{m} \left(T - \left\langle \frac{p^2}{2m} \right\rangle \right)$$

- Average power absorbed by the particle

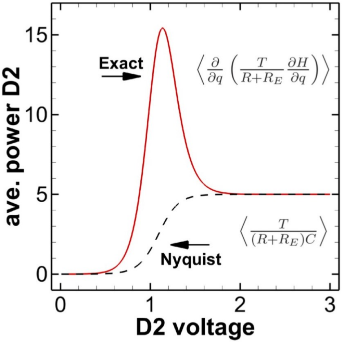
$$\left\langle \frac{\mathrm{d}' W}{\mathrm{d}t} \right\rangle = \left\langle \frac{\partial}{\partial q} \left(\frac{T}{\mathcal{R}} \frac{\partial \mathcal{H}}{\partial q} \right) \right\rangle - \left\langle \frac{1}{\mathcal{R}} \left(\frac{\partial \mathcal{H}}{\partial q} \right)^2 \right\rangle$$

Quantities used for Simulation

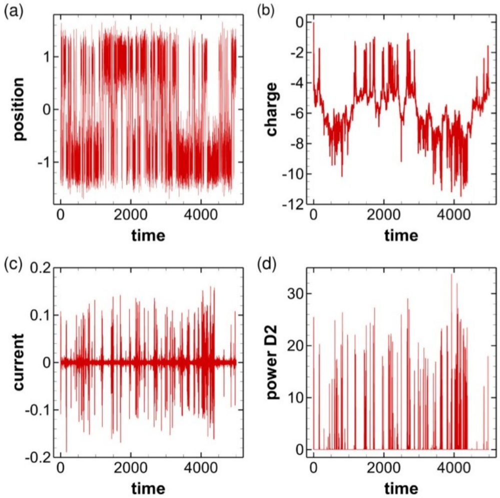
- Ripple Height, $l = 1\,nm$
- Distance between graphene and STM Tip, $d = 10l$
- Acoustic Phonon Frequency, $\eta/m = 1\,THz$
- Saturation Current, $I_0 = 1\,nA$
- Capacitance for Tip-Graphene Junction, $C_0 = 1\,fF$

Simulation

- Nyquist result vs Exact Result



Simulation


(a)
position
time
1
0
-1
0
2000
4000
(b)
charge
time
0
-2
-4
-6
-8
-10
-12
(c)
current
time
0.2
0.1
0
-0.1
-0.2
(d)
power D2
time
30
20
10

Simulation

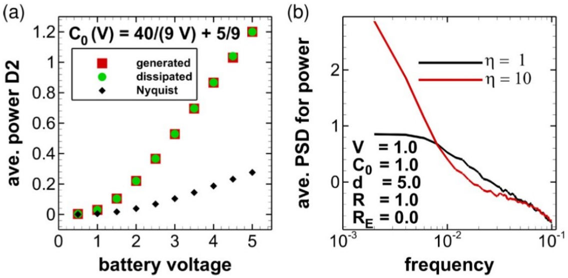


FIG. 6. Ito-Langevin equation simulation results for a circuit with diodes and resistor. (a) Average counterclockwise power versus battery voltage. (b) Average power spectrum density of power vs. frequency.

Equilibrium Average of Generated Power

- *“The overall equilibrium power due to the electric circuit is zero because the dissipated power at diodes and resistor are compensated exactly by the power generated by thermal fluctuations”*