4th International Electronic Conference on Entropy and Its Applications (21/11 - 1/12, 2017)

Clausius relation for Active Particles

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A. Puglisi and U. Marini Bettolo Marconi, Entropy 19, 356 (2017)
U. Marini Bettolo Marconi, A.Puglisi, C.Maggi, Scientific Reports 7, 46496 (2017)

Clausius relation in macroscopic thermodynamics

δQ Is the heat exchanged with the thermostat during a transformation

$$\delta\Sigma = dS - \frac{\delta Q}{T} \geq 0$$

Is the entropy production

$$\oint \frac{\delta Q(t)}{T(t)} \leq 0$$

Is the **Clausius relation** for a cyclical transformation

Mesoscopic description

$\{\omega(t')\}_0^t$ Is a stochastic trajectory

$$\ln \frac{\text{prob}[\{\omega(t')\}_0^t]}{\text{prob}[\{\overline{\omega}(t-t')\}_0^t]} = \ln \frac{p[\omega(0)]}{p[\overline{\omega(t)}]} + \ln \frac{\text{prob}[\{\omega(t')\}_0^t|\omega(0)]}{\text{prob}[\{\overline{\omega}(t-t')\}_0^t|\overline{\omega}(t)]}$$

$$\int_0^t \delta\sigma(t') = \int_0^t ds + \int_0^t \delta s_m$$

$$\delta s_m = -\delta q/T$$

Steady state averages

$$\delta\Sigma = \langle\delta\sigma\rangle \geq 0 \qquad dS = \langle ds\rangle \qquad \langle\delta s_m\rangle = -\delta Q/T \geq 0$$

A simple example

$$dx(t) = u(t)dt$$

$$mdu(t) = -\gamma u(t)dt + \sqrt{2\gamma T}dW(t) - \phi'[x(t)]dt + f_{nc}(t)dt$$

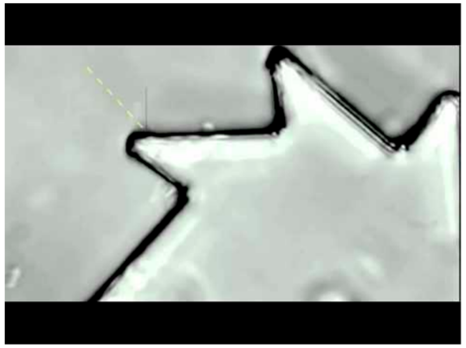
$$e = \frac{mu^2}{2} + \phi(x)$$

$$\delta w = u f_{nc} dt \qquad \delta q = de - \delta w = u \circ [-\gamma u dt + \sqrt{2\gamma T}dW(t)]$$

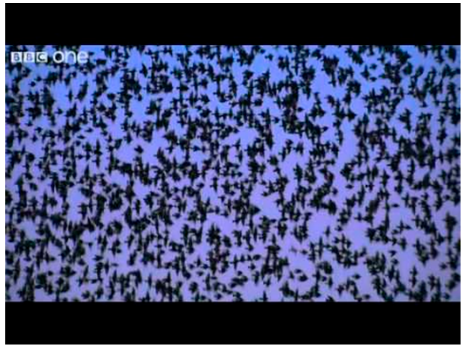
$$\delta\sigma = ds - \frac{u \circ [-\gamma u dt + \sqrt{2\gamma T}dW]}{T} = \boxed{ds - \frac{\delta q}{T}}$$

Active particles

Self-propulsion



Bacteria driving a motor



Swarming birds

A stochastic active model

$$dx(t) = u(t)dt$$

$$mdu(t) = -\gamma u(t)dt + \sqrt{2\gamma T_b}dW(t) + f_a(t)dt - \phi'[x(t)]dt$$

$$df_a(t) = -\frac{f_a(t)}{\tau}dt + \frac{\gamma\sqrt{2D_a}}{\tau}dW_2(t) \qquad T_a = \gamma D_a$$

$$dx(t) = \frac{\sqrt{2\gamma T_b}dW(t) + f_a(t)dt - \phi'[x(t)]dt}{\gamma}$$

Heat into the solvent

$$\delta w = u f_a dt \qquad \delta q_b = u \circ \left[-\gamma u dt + \sqrt{2\gamma T_b} dW(t)\right]$$

$$\delta\sigma = ds - \frac{\delta q_b}{T}$$

$$Q_b = \langle q_b \rangle \Longrightarrow \boxed{\frac{\delta Q_b}{T} \leq 0}$$

Steady state

Neglecting thermal noise

$$\dot{x} = \frac{f_a(t) - \phi'(x)}{\gamma}$$

$$dx(t) = u(t)dt$$

$$\mu du(t) = -\gamma u(t)dt + \sqrt{2\gamma T_a}dW(t) - \phi'[x(t)]dt - \tau\phi''[x(t)]u(t)dt$$

$$= -\gamma\Gamma(x)u(t)dt + \sqrt{2\gamma\Gamma(x)\theta(x)}dW(t) - \phi'[x(t)]dt$$

$$\mu = \gamma\tau \qquad \Gamma(x) = 1 + \frac{\tau}{\gamma}\phi''(x) \qquad \theta(x) = T_a/\Gamma(x)$$

Entropy production

$$\boxed{\delta q_{ab} = u \circ df_{ab}}$$

$$\delta\sigma = ds - \frac{\delta q_{ab}}{\theta(x)}$$

$$df_{ab}(t) = -\gamma\Gamma[x(t)]u(t)dt + \sqrt{2\gamma\Gamma[x(t)]\theta(x)}dW(t)$$

Power exchanged with the
active heat-bath at temperature $\theta(x)$

Clausius relation for active particles

In the steady state

$$\left\langle \frac{\delta q_{ab}(x)}{\theta(x)} \right\rangle \leq 0$$

$$\left\langle \frac{\delta q_{ab}(x)}{\theta(x)} \right\rangle = \int dx \frac{\dot{\tilde{q}}(x)}{\theta(x)}$$

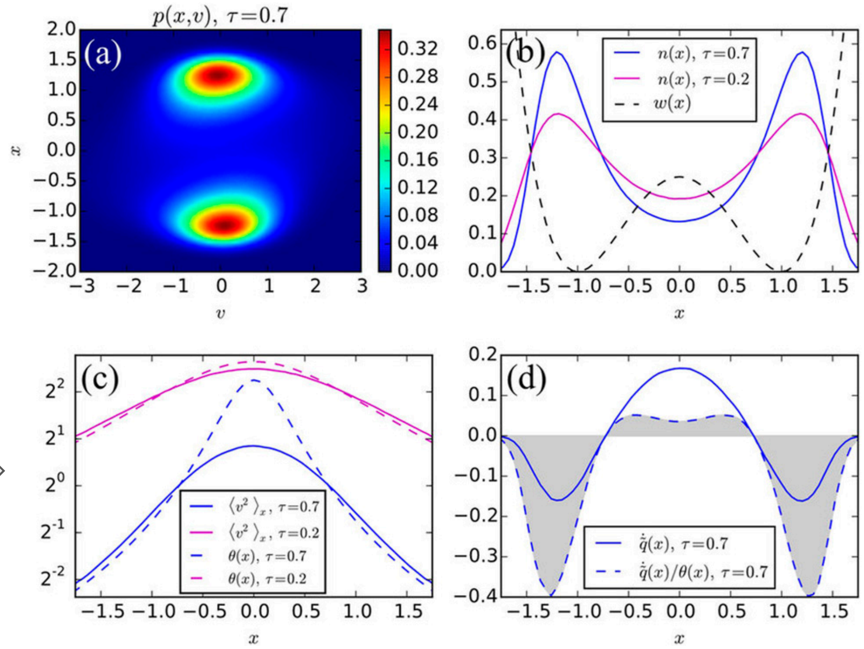
$$\dot{\tilde{q}}(x) = \gamma\Gamma(x) \left[\frac{\theta(x)}{\mu} n(x) - \int dv u^2 p(x,u) \right]$$

An example

$$w(x) \equiv \phi(x) = \frac{x^4}{4} - \frac{x^2}{2}$$

Probability density in x,u

Number density and potential



Kinetic and effective temperatures

Heat flux density, entropy production density and its integral

In more than 1 dimension

$$\mu du_i = -\gamma \Gamma_{ij}(\mathbf{r}) u_j dt - \partial_i \phi(\mathbf{r}) dt + \gamma \sqrt{2D_a} dW_i$$

$$\Gamma_{ij} = \delta_{ij} + \frac{\tau}{\gamma} \partial_j \partial_i \phi$$

$$P \Gamma P^T = D \qquad D_{ij}(\mathbf{r}) = \lambda_i(\mathbf{r}) \delta_{ij}$$

$$\delta\sigma(t) = ds(t) - \sum_i \frac{\delta q_{ab,i}(t)}{\theta_i[\mathbf{R}(t)]} \qquad \theta_i(\mathbf{R}) = T_a / \lambda_i(\mathbf{R})$$

$$\delta q_{ab,i} = U_i \circ [-\gamma \lambda_i(\mathbf{R}) U_i dt + \gamma \sqrt{2D_a} dW]$$

Thanks for your attention!