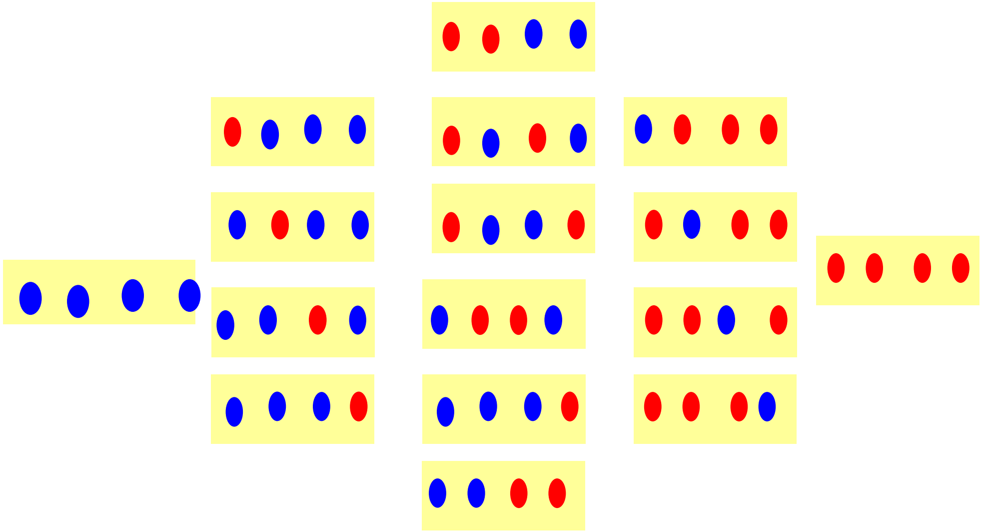
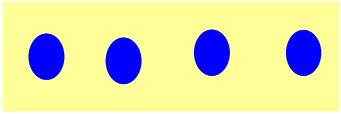
** Origin of entropic forces

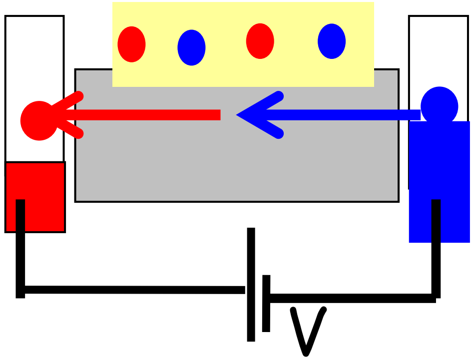




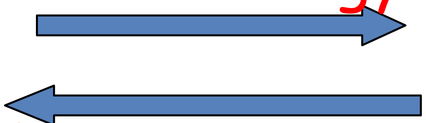
S = k log W

W = 2^N, S = Nk ln2

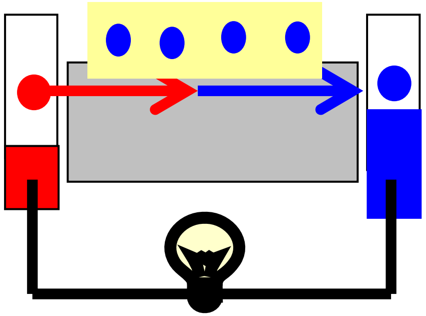
S = 0, W = 1



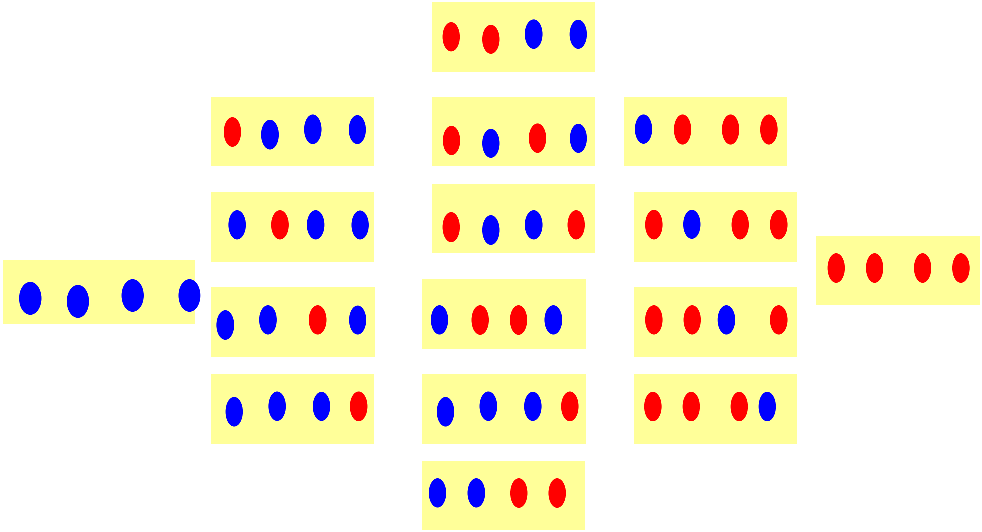
Need energy



Gives up energy



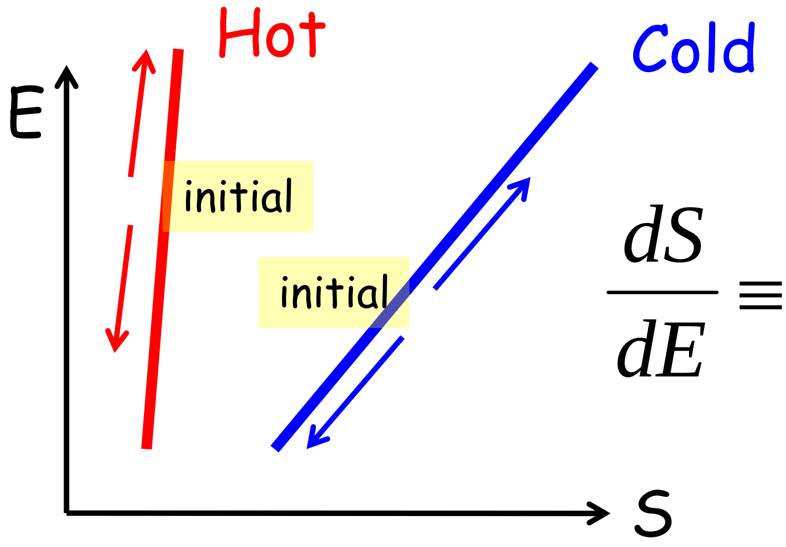
Temperature



$$S = k \log W$$

$$\approx \; -k \sum_i P_i \ln P_i$$

$$P_i \sim \; \exp(-\varepsilon_i / kT)$$



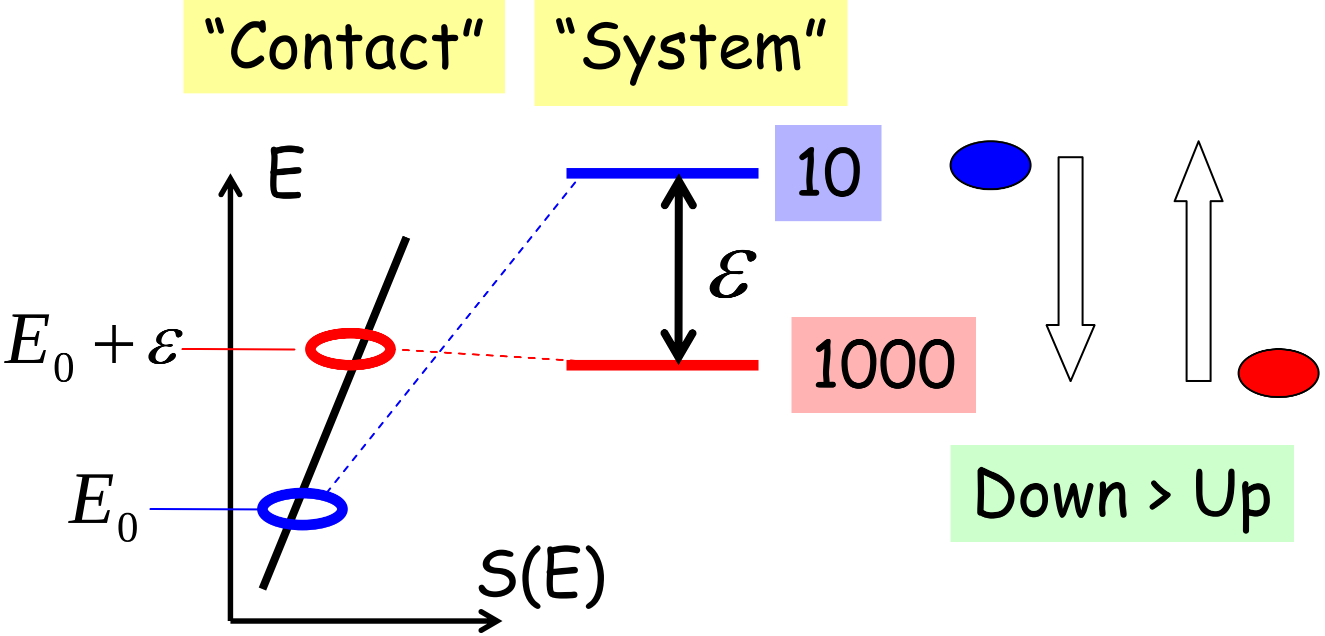
$$\frac{dS}{dE} \equiv \frac{1}{T}$$

Second Law:

$S_{final} > S_{initial}$

$W_{final} > W_{initial}$

Modeling the entropic "force"



$$\frac{Down}{Up} = \frac{W(E_0+\varepsilon)}{W(E_0)} = \exp\left(\frac{S(E_0+\varepsilon)-S(E_0)}{k}\right) = exp\left(\frac{\varepsilon}{kT}\right)$$

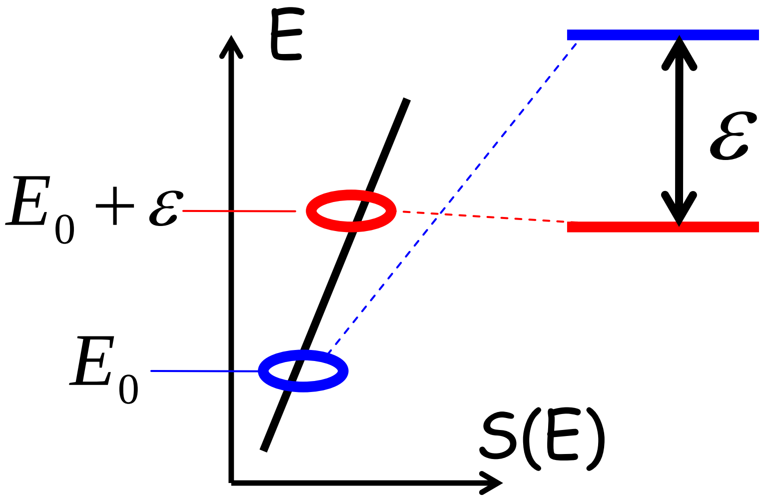
$$S \sim k\log W$$

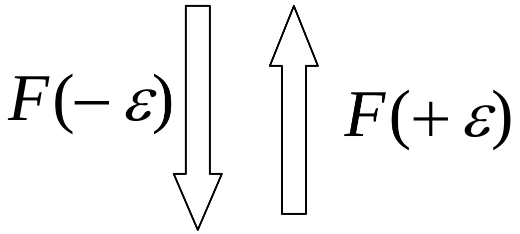
$$\rightarrow W \sim \exp(S/k)$$

$$S(E_0+\varepsilon)-S(E_0) \approx \frac{dS}{dE}\varepsilon = \frac{\varepsilon}{T}$$

Modeling the entropic "force"

"Contact" "System"





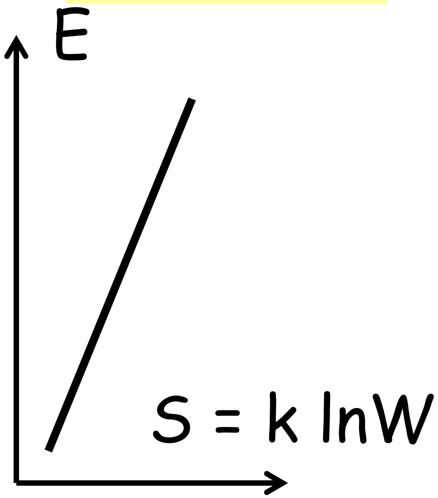
Down > Up

$$\frac{F(-\varepsilon)}{F(+\varepsilon)} = \frac{W(E_0+\varepsilon)}{W(E_0)}$$

$$= exp\left(\frac{\varepsilon}{kT}\right)$$

“Density of states”

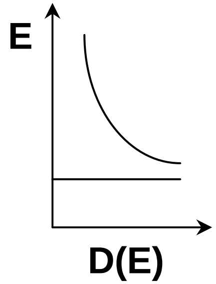
“Contact”



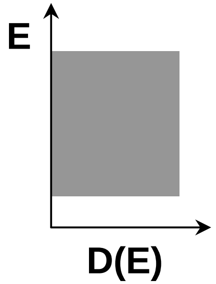
Need to consider 3N dimensions: See Feynman, Statistical Mechanics, Chapter 1

Electrons with effective mass ‘m’

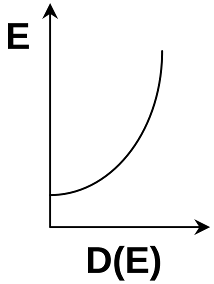
$$1D: \quad D \quad \sim \quad 1/\sqrt{E}$$



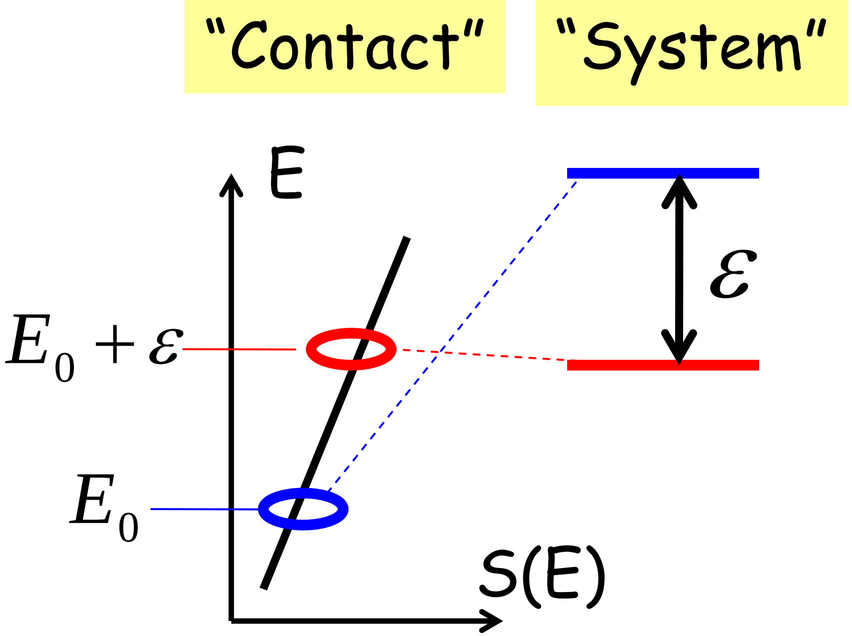
$$2D: \quad D \quad \sim \quad E^{0}$$

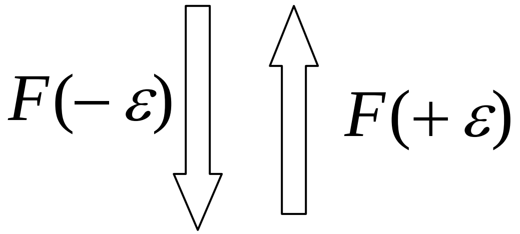


$$3D: \quad D \quad \sim \quad \sqrt{E}$$



Modeling the entropic "force"





Down > Up

$$\frac{F(-\varepsilon)}{F(+\varepsilon)} = \frac{W(E_0+\varepsilon)}{W(E_0)}$$

$$= exp\left(\frac{\varepsilon}{kT}\right)$$

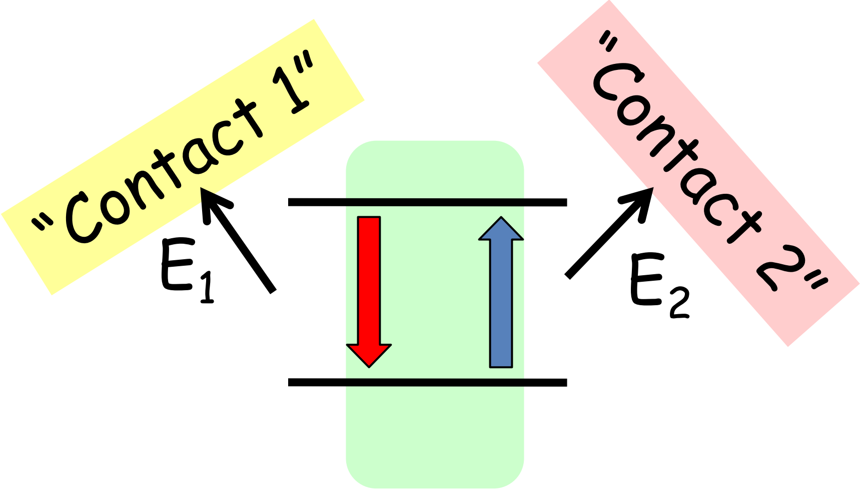
<u>For any "contact" in equilibrium</u>

Easier to give energy to it,

than to extract energy from it.

Second law

$$E_1 + E_2 = 0$$



$$\frac{F(-E)}{F(E)} = \frac{W(E_C + E)}{W(E_C)}$$

$$= \exp\left(\frac{E}{kT_C}\right)$$

$$S \sim k \log W$$

$$\rightarrow W \sim \exp(S/k)$$

$$\frac{F_1(-E_1)\, F_2(-E_2)}{F_1(E_1)\, F_2(E_2)} > 1$$

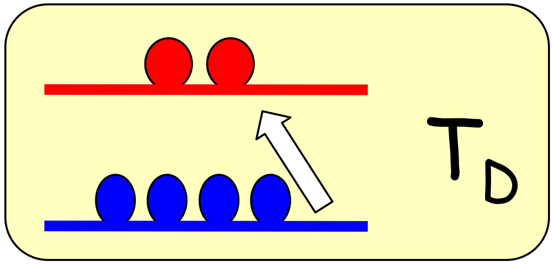
$$\exp\left(\frac{E_1}{kT_1}\right) \exp\left(\frac{E_2}{kT_2}\right) > 1$$

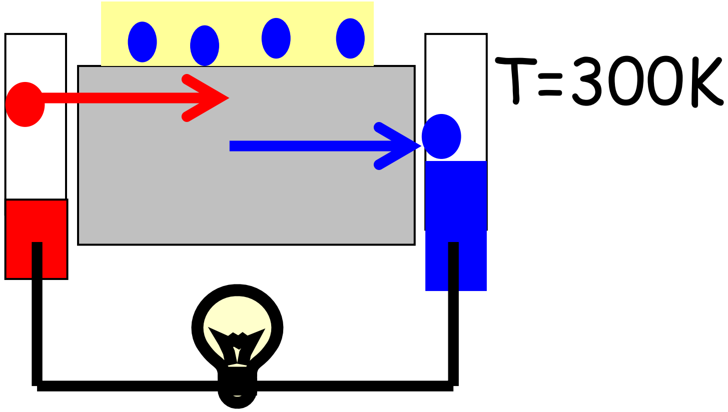
$$\frac{E_1}{kT_1} + \frac{E_2}{kT_2} > 0$$

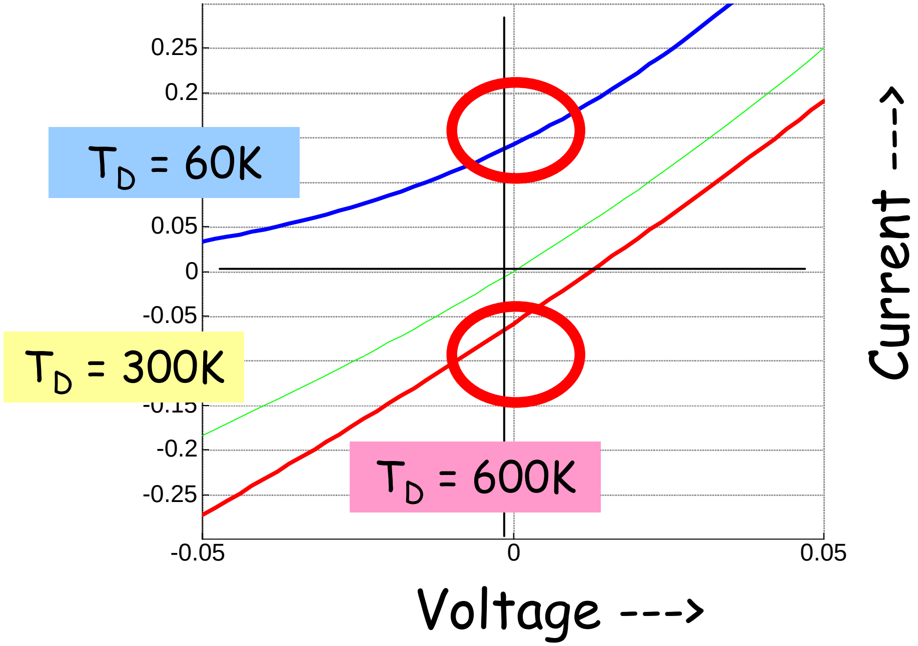
$$\sum_i E_i = 0$$

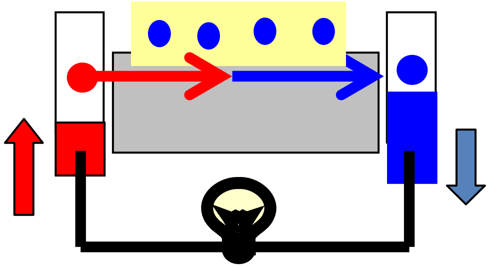
$$\sum_i \frac{E_i - \mu_i}{T_i} \leq 0$$

A heat engine



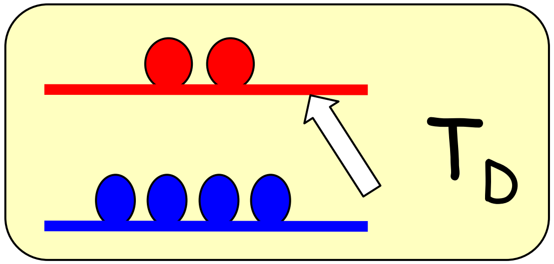




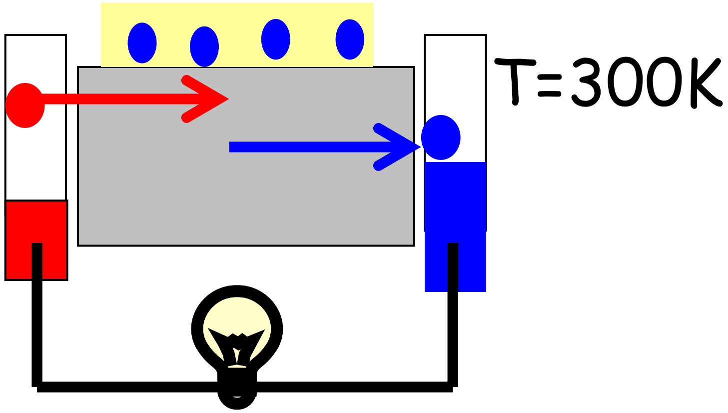


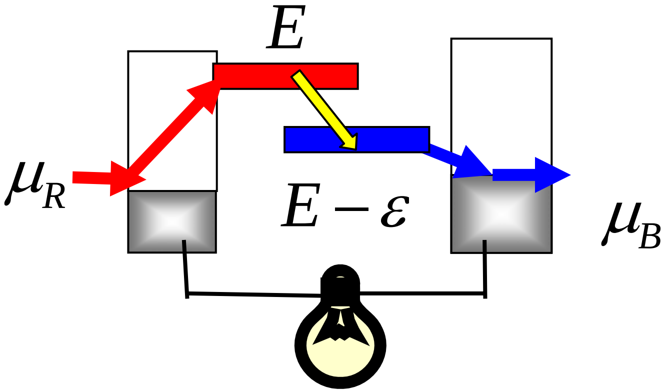
Cf. Feynman lectures,
Vol.1, Ratchet and pawl

Analyzing the heat engine



$$\frac{F_{BR}(-\varepsilon)}{F_{RB}(+\varepsilon)} = \exp\left(\frac{\varepsilon}{kT_D}\right)$$



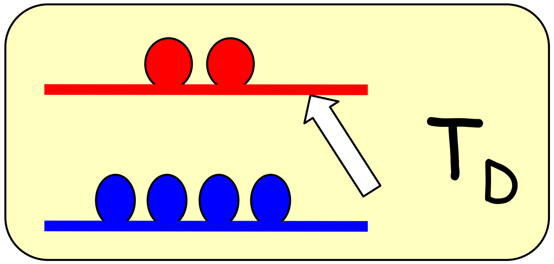


$$I_s \sim \quad F_{B\leftarrow R}(-\varepsilon) \quad n_R(E) \quad p_B(E-\varepsilon)$$

minus

$$F_{R\leftarrow B}(+\varepsilon) \quad n_B(E-\varepsilon) \quad p_R(E)$$

Analyzing the heat engine ..

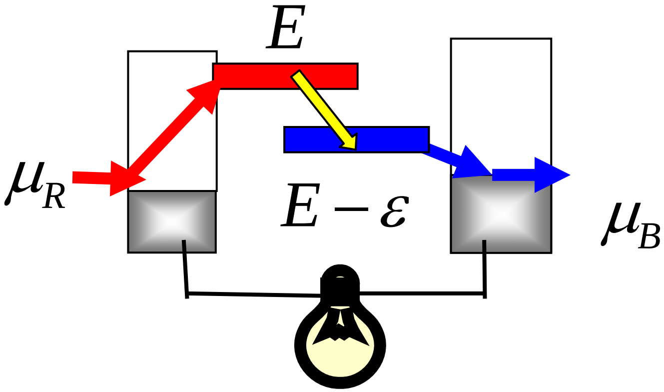


$$\frac{F_{BR}(-\varepsilon)}{F_{RB}(+\varepsilon)} = \exp\left(\frac{\varepsilon}{kT_D}\right)$$

$$\frac{F_{BR}(-h\omega)}{F_{RB}(+h\omega)} = \exp\left(\frac{h\omega}{kT_D}\right)$$

$$Is \quad \frac{N(\omega)+1}{N(\omega)} = \exp\left(\frac{h\omega}{kT_D}\right) \quad ?$$

$$Yes, \quad if \quad N(\omega) = \frac{1}{\exp\left(\frac{h\omega}{kT_D}\right)-1}$$

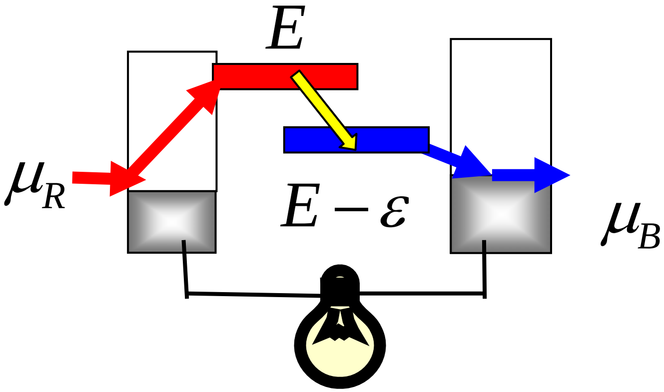


$$I_s \sim \quad F_{B\leftarrow R}(-\varepsilon) \quad n_R(E) \quad p_B(E-\varepsilon)$$

minus

$$F_{R\leftarrow B}(+\varepsilon) \quad n_B(E-\varepsilon) \quad p_R(E)$$

Entropic forces in NEGF



$$I_s \sim \quad F_{B\leftarrow R}(-\varepsilon) \quad n_R(E) \quad p_B(E-\varepsilon)$$

minus

$$F_{R\leftarrow B}(+\varepsilon) \quad n_B(E-\varepsilon) \quad p_R(E)$$

$$\begin{pmatrix} n_R \\ n_B \end{pmatrix} \rightarrow \left[G^n\right]$$

$$\frac{F_{BR}(-\varepsilon)}{F_{RB}(+\varepsilon)} = \exp\left(\frac{\varepsilon}{kT_D}\right)$$

$$\begin{pmatrix} p_R \\ p_B \end{pmatrix} \rightarrow \left[G^p\right]$$

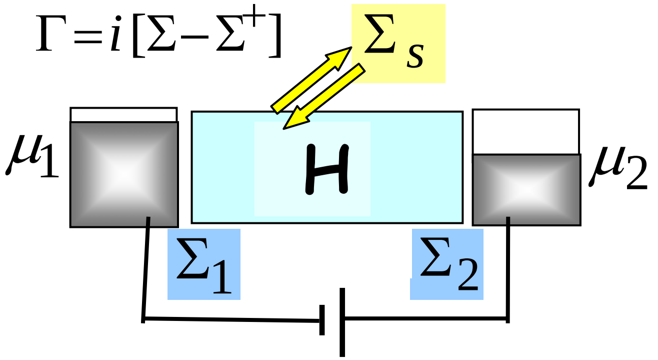
$$n+p=DOS$$

$$\rightarrow \left[G^n\right]+\left[G^p\right]=[A]$$

$$\frac{D_{ijkl}(-\varepsilon)}{D_{lkji}(+\varepsilon)} = \exp\left(\frac{\varepsilon}{k_B T_D}\right)$$

NEGF equations for elastic scatterers in equilibrium

$$\Gamma = i[\Sigma - \Sigma^+]$$



Green function

$$[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$$

"Electron density"

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1 + G\Sigma_s^{in} G^+$$

"Hole density"

$$G^p = G\Gamma_2 G^+ (1 - f_2) + G\Gamma_1 G^+ (1 - f_1) + G\Sigma_s^{out} G^+$$

"Density of states"

$$A = G^n + G^p$$
$$= i[G - G^+]$$

Dephasing

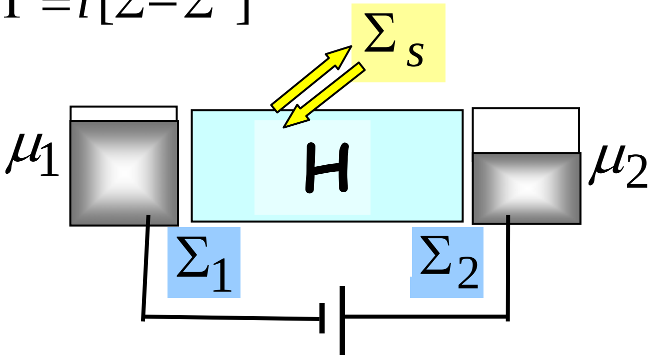
$$[\Sigma_s^{in}] = D[G^n]$$
$$[\Sigma_s] = D[G]$$
$$\Sigma_s^{out} = D[G^p]$$

Broadening

$$[\Gamma_s] = \left[\Sigma_s^{in} + \Sigma_s^{out}\right]$$
$$= i[\Sigma_s - \Sigma_s^+]$$

Energy exchange in NEGF

$\Gamma = i\,[\Sigma - \Sigma^{+}]$



$$\left[D^p(\varepsilon)\right]_{ijkl} = \left[D(-\varepsilon)\right]_{lkji}$$

Dephasing, general

$$[\Sigma_s^{in}(E)] = D(+\varepsilon)\,[G^n(E-\varepsilon)]$$

$$[\Sigma_s^{out}(E)] = D^p(\varepsilon)\,[G^p(E-\varepsilon)]$$

$$[\Gamma_s(E)] = \left[\Sigma_s^{in}(E) + \Sigma_s^{out}(E\right]$$

$$[\Sigma_s(E)] = [h(E)] - \frac{i}{2}\left[\Gamma_s(E)\right]$$

"Density of states"

$$A = G^n + G^p$$

$$= i[G - G^{+}]$$

Elastic Dephasing

$$[\Sigma_s^{in}(E)] = D\,[G^n(E)]$$

$$\cancel{[\Sigma}_s(E)] = D\,[G(E)]$$

$$\Sigma_s^{out}(E) = \cancel{D}[G^p(E)]$$

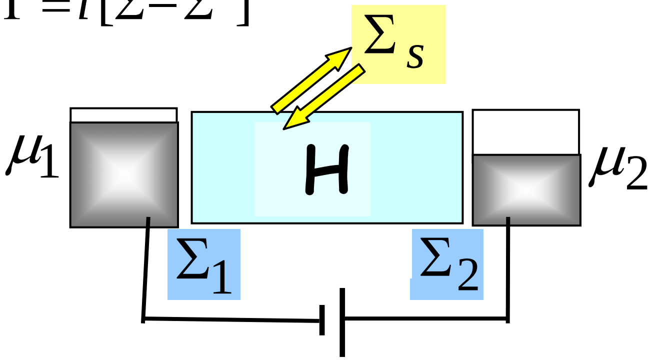
Broadening

$$[\Gamma_s] = \left[\Sigma_s^{in} + \Sigma_s^{out}\right]$$

$$= i\,[\Sigma_s - \Sigma_s^{+}]$$

Energy exchange in NEGF

$\Gamma = i[\Sigma - \Sigma^{+}]$



Energy exchange

$$[\Sigma_s^{in}(E)] = D(\varepsilon)[G^n(E-\varepsilon)]$$

$$[\Sigma_s^{out}(E)] = D^p(\varepsilon)[G^p(E-\varepsilon)]$$

$$[\Gamma_s(E)] = \left[\Sigma_s^{in}(E) + \Sigma_s^{out}(E\right]$$

$$[\Sigma_s(E)] = [h(E)] - \frac{i}{2}\left[\Gamma_s(E)\right]$$

$$\left[D^p(\varepsilon)\right]_{ijkl} = \left[D(-\varepsilon)\right]_{lkji}$$

"Density of states"

$$A = G^n + G^p$$

$$= i[G - G^{+}]$$

For scatterers in equlibriun

$$\frac{D_{ijkl}(-\varepsilon)}{D_{lkji}(+\varepsilon)} = \exp\left(\frac{\varepsilon}{k_B T_D}\right)$$

Like semiclassical theory .. sort of ..

$$[\Sigma_s^{in}(E)] \;=\; D(\varepsilon)\,[G^n(E-\varepsilon)]$$

$$[\Sigma_s^{out}(E)] \;=\; D^p(\varepsilon)\,[G^p(E-\varepsilon)]$$

$$\frac{I_1}{q/h} \sim \quad Trace[G^p(E)\,\Sigma_1^{in}(E)$$

$$\text{minus} \quad G^n(E)\,\Sigma_1^{out}(E)]$$

$$\left[\left[D^p(\varepsilon)\right]\right] \;=\; \left[\left[D(-\varepsilon)\right]\right]^T$$

$$\left[D^p(\varepsilon)\right]_{ijkl} \;=\; \left[D(-\varepsilon)\right]_{lkji}$$

$$\frac{dN}{dt} \sim \{p(E)\}^T \overbrace{[F(+\varepsilon)]\{n(E-\varepsilon)\}}$$

$$\text{minus}\{n(E)\}^T \underbrace{[F(-\varepsilon)]^T\{p(E-\varepsilon)\}}$$

$$[\Sigma_s^{in}(E)] \;=\; \left[\left[D(\varepsilon)\right]\right][G^n(E-\varepsilon)]$$

$$[\Sigma_s^{out}(E)] \;=\; \left[\left[D(-\varepsilon)\right]\right]^T\,[G^p(E-\varepsilon)]$$

$$\frac{d\,n_R}{d\,t} \sim \quad F_{RB}(+\varepsilon) \quad n_B(E-\varepsilon) \quad p_R(E)$$

$$\text{minus} \quad F_{BR}(-\varepsilon) \quad n_R(E) \quad p_B(E-\varepsilon)$$

Like semiclassical theory .. sort of ..

"Demon" in equilibrium

$$\frac{F_{BR}(-\varepsilon)}{F_{RB}(+\varepsilon)} = \exp\left(\frac{\varepsilon}{kT_D}\right)$$

$$\frac{[F(-\varepsilon)]_{BR}}{[F(+\varepsilon)]^T{}_{BR}} = \exp\left(\frac{\varepsilon}{kT_D}\right)$$

$$\frac{D_{ijkl}(-\varepsilon)}{D_{lkji}(+\varepsilon)} = \exp\left(\frac{\varepsilon}{kT_D}\right)$$

$$[\Sigma_s^{in}(E)] = D(\varepsilon)\,[G^n(E-\varepsilon)]$$

$$[\Sigma_s^{out}(E)] = D^p(\varepsilon)\,[G^p(E-\varepsilon)]$$

$$[[D^p(\varepsilon)]] = [[D(-\varepsilon)]]^T$$

$$\frac{dN}{dt} \sim \{p(E)\}^T \overbrace{[F(+\varepsilon)]\{n(E-\varepsilon)\}}$$

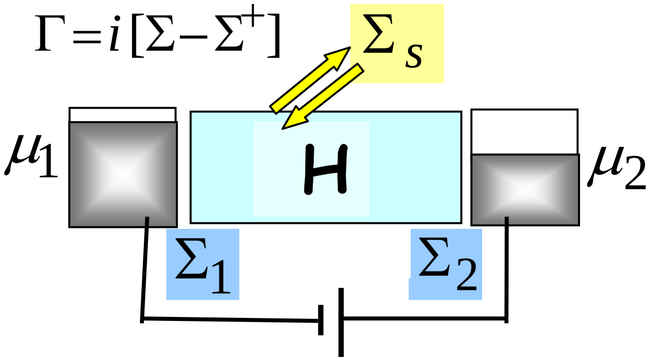
$$\text{minus}\{n(E)\}^T \underbrace{[F(-\varepsilon)]^T\{p(E-\varepsilon)\}}$$

$$[\Sigma_s^{in}(E)] = [[D(\varepsilon)]][G^n(E-\varepsilon)]$$

$$[\Sigma_s^{out}(E)] = [[D(-\varepsilon)]]^T\,[G^p(E-\varepsilon)]$$

NEGF equations .. including "everything" .. almost ..

$$\Gamma = i[\Sigma - \Sigma^{+}]$$



Green function

$$[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$$

"Electron density"

$$G^n = G\Gamma_2 G^{+} f_2 + G\Gamma_1 G^{+} f_1 + G\Sigma_s^{in} G^{+}$$

"Hole density"

$$G^p = G\Gamma_2 G^{+}(1 - f_2) + G\Gamma_1 G^{+}(1 - f_1) + G\Sigma_s^{out} G^{+}$$

"Density of states"

$$A = G^n + G^p$$
$$= i[G - G^{+}]$$

Current

$$\frac{I_1}{q/\hbar} = Trace\left([\Gamma_1 A]\, f_1 - [\Gamma_1 G^n]\right)$$

Broadening

$$[\Gamma_s] = \left[\Sigma_s^{in} + \Sigma_s^{out}\right]$$
$$= i\,[\Sigma_s - \Sigma_s^{+}]$$

Energy exchange

$$[\Sigma_s^{in}(E)] = \left[\left[D(\varepsilon)\right]\right] [G^n(E-\varepsilon)]$$

$$[\Sigma_s^{out}(E)] = \left[\left[D(-\varepsilon)\right]\right]^T [G^p(E-\varepsilon)]$$

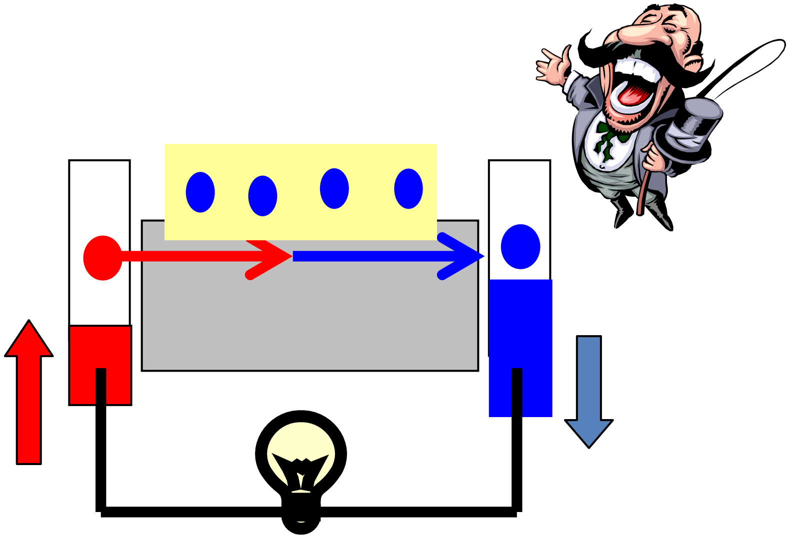
$$[\Sigma_s(E)] = [h(E)] - \frac{i}{2}\left[\Gamma_s(E)\right]$$

NCN

http://www.nanohub.org/courses/cqt

Supriyo Datta

“Contacts” not in equilibrium



Semiclassical

$$\frac{F_{BR}(-\varepsilon)}{F_{RB}(+\varepsilon)} = \exp\left(\frac{\varepsilon}{kT_C}\right)$$

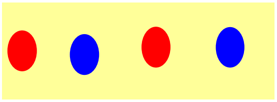
NEGF

$$\frac{D_{ijkl}(-\varepsilon)}{D_{lkji}(+\varepsilon)} = \exp\left(\frac{\varepsilon}{k_B T_C}\right)$$

$$\frac{F_{B\leftarrow R}(\varepsilon=0)}{F_{R\leftarrow B}(\varepsilon=0)} = \frac{1}{0} \rightarrow \infty$$

.. can be handled if we know the state of the scatterer ..

$$\exp\left(\frac{\varepsilon\rightarrow 0}{kT_C}\right) = 1$$



Scatterers driven off equilibrium

Non-interacting spins:
Bloch equation

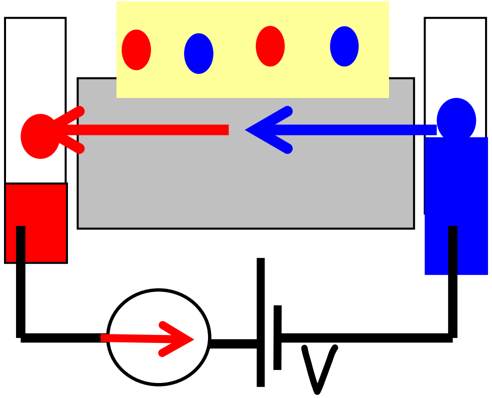
$$\frac{\partial \vec{m}}{\partial t} = \gamma(\vec{m} x \vec{H})$$

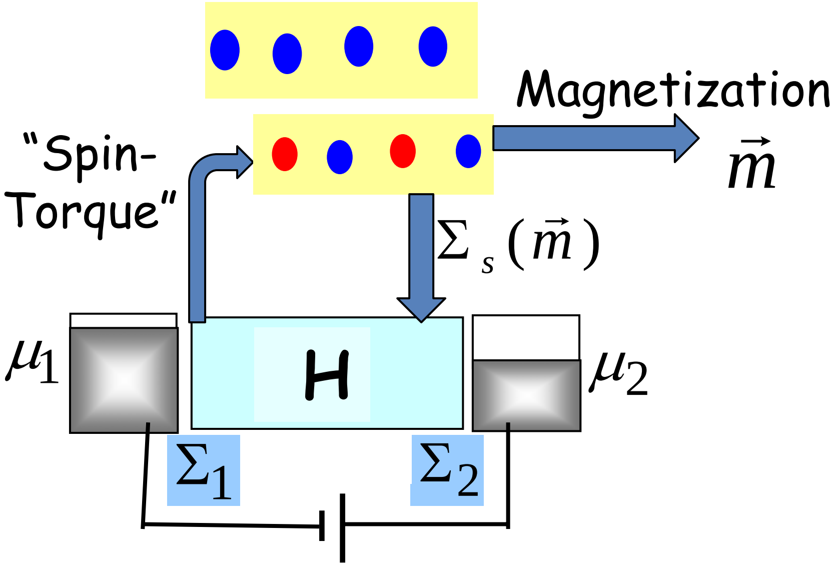
$$-\frac{\vec{m}-\vec{m}_0}{T}$$

Damping

$$+\vec{T}$$

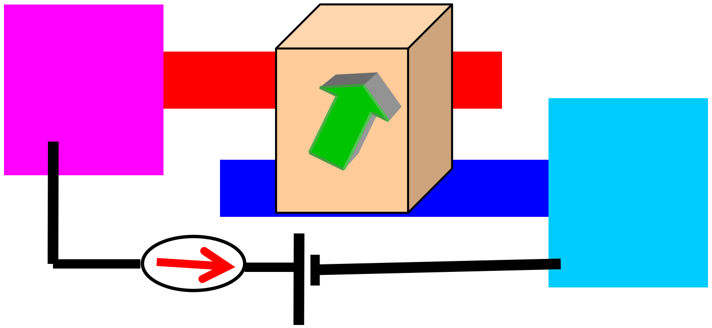
"Spin-Torque"





Scatterers driven off equilibrium

Nanomagnets: LLG equation



$$(1+\alpha^2)\frac{\partial\vec{m}}{\partial t}=\gamma(\vec{m}x\vec{H})$$

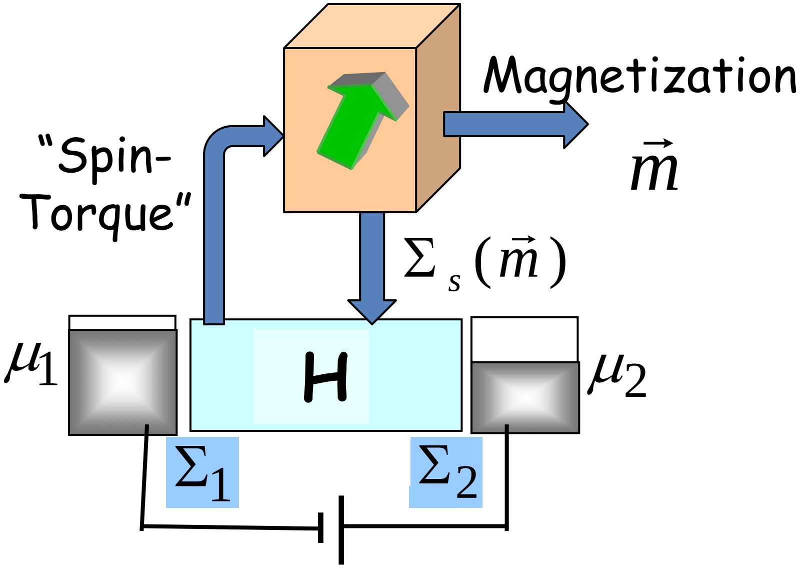
$$-\frac{\gamma\alpha}{m}(\vec{m}x\vec{m}x\vec{H})$$

Gilbert damping

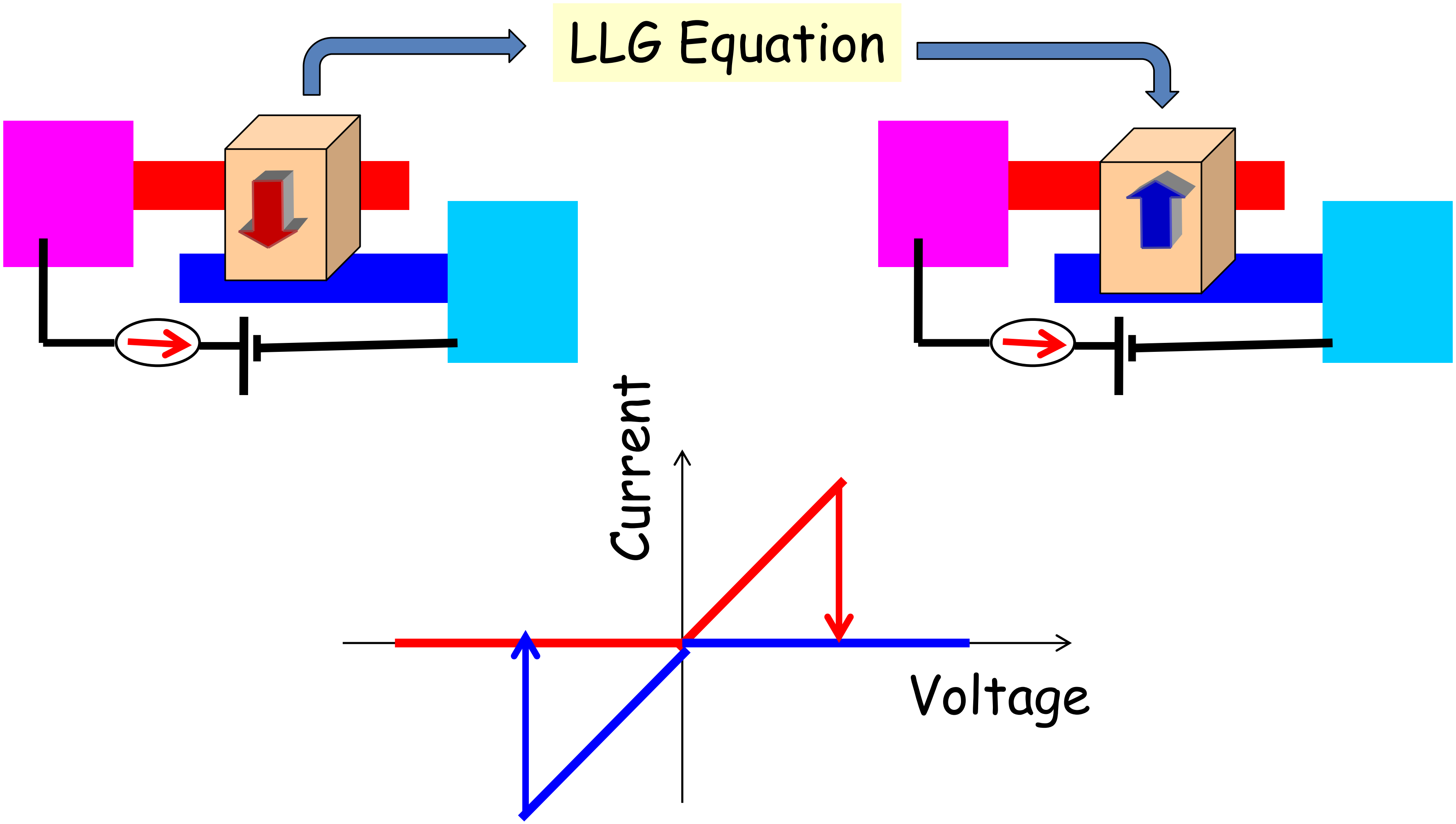
$$+\vec{T}$$

" Spin-Torque"

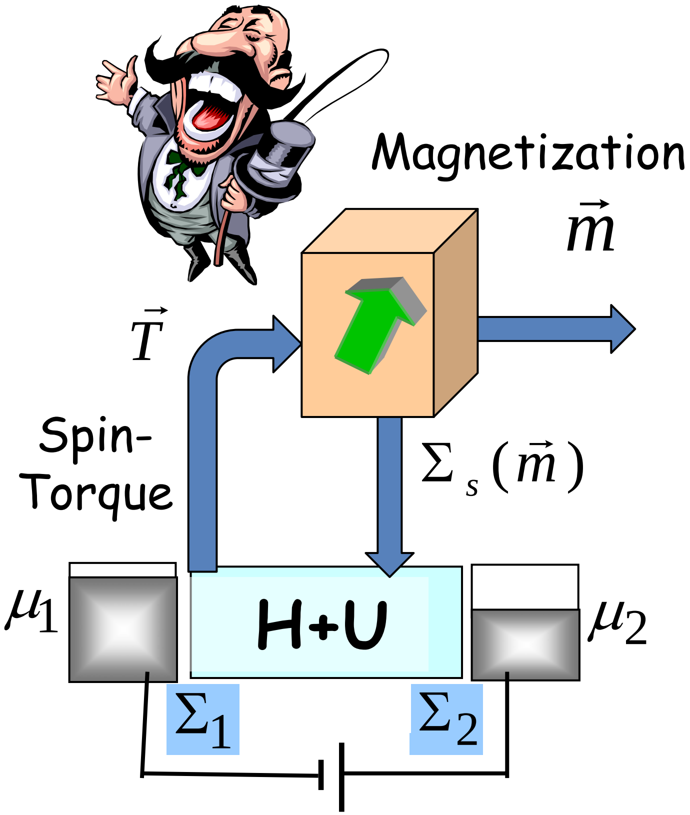
$$\vec{H}=\vec{H}_{ext}+\vec{H}_{\text{int}}(\vec{m})$$



Bistable “contacts”



Classifying demons



No demon .. just source/drain

Rigid demon .. gates

Elastic demon .. in equilibrium

Inelastic demon .. in equilibrium

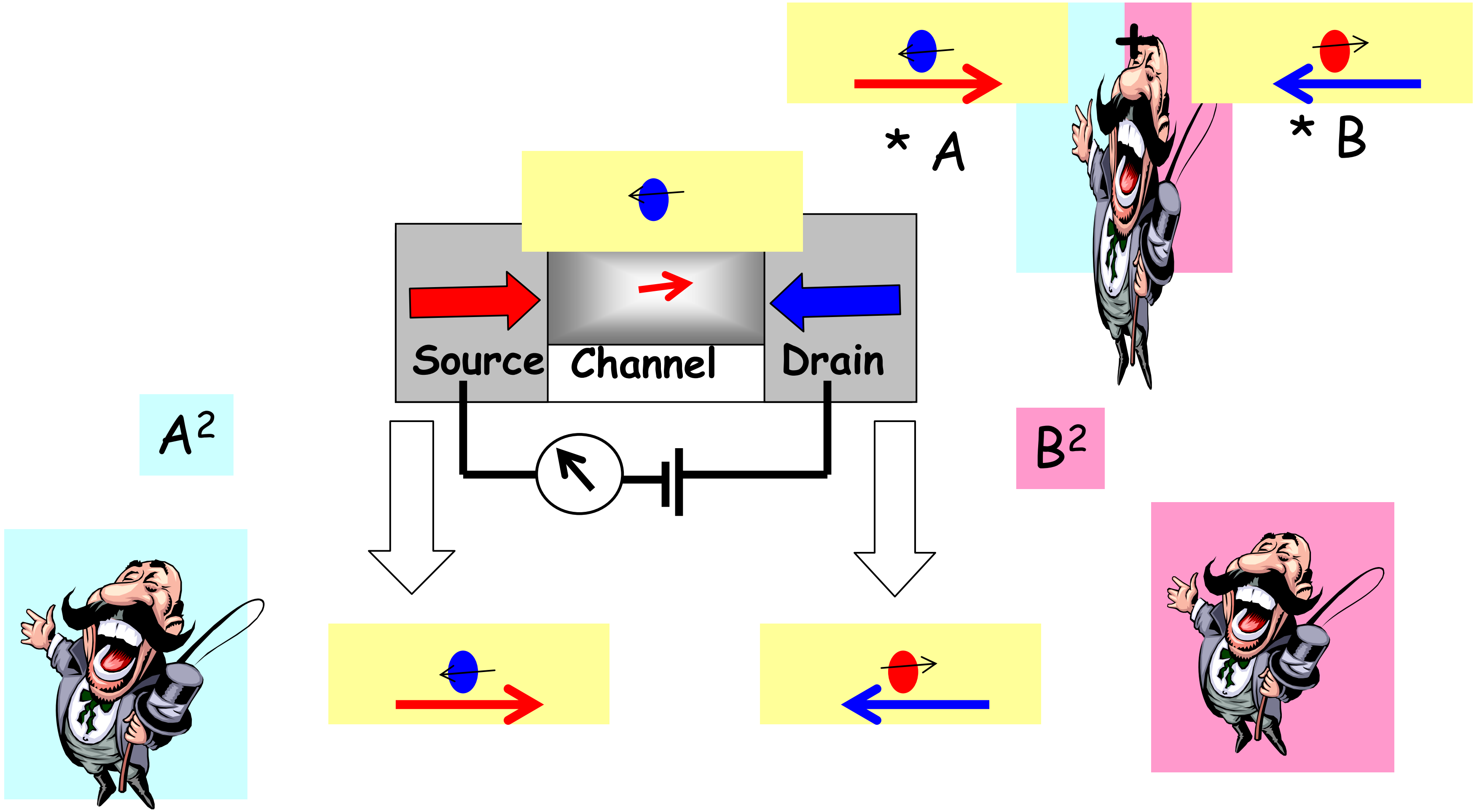
Elastic demon .. out-of-equilibrium

Inelastic demon .. out-of-equilibrium

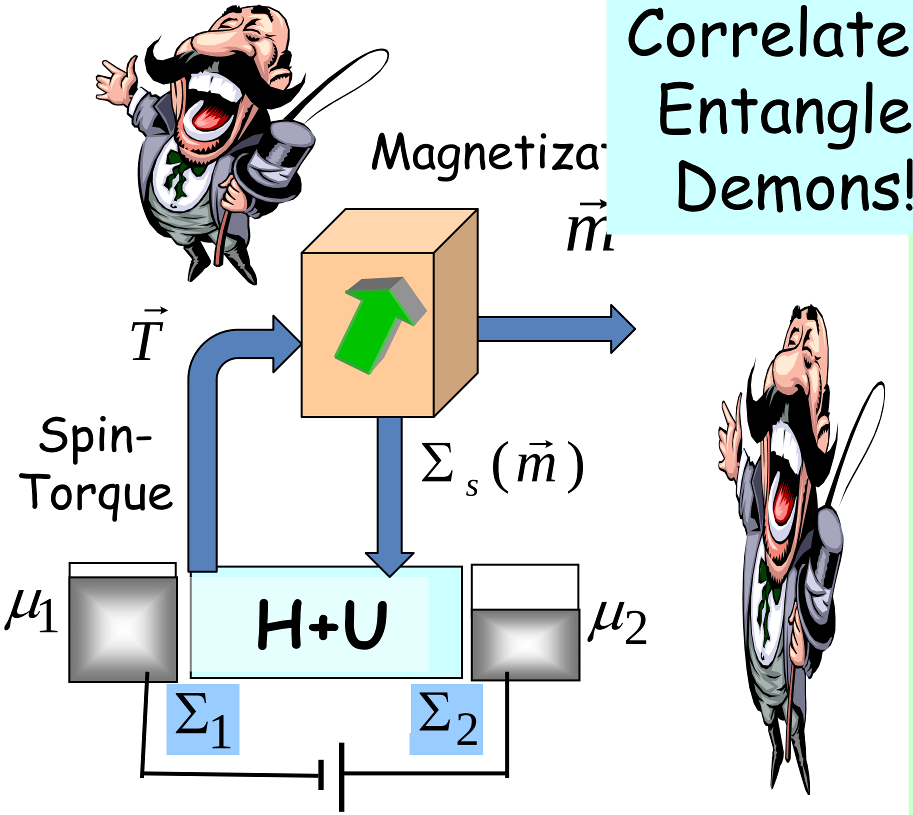
Bistable demon

** Entangled Demon

Entangled !



Classifying demons



Correlated/
Entangled
Demons!!

No demon .. just source/drain

Rigid demon .. gates

Elastic demon .. in equilibrium

Inelastic demon .. in equilibrium

Elastic demon .. out-of-equilibrium

Inelastic demon .. out-of-equilibrium

Bistable demon