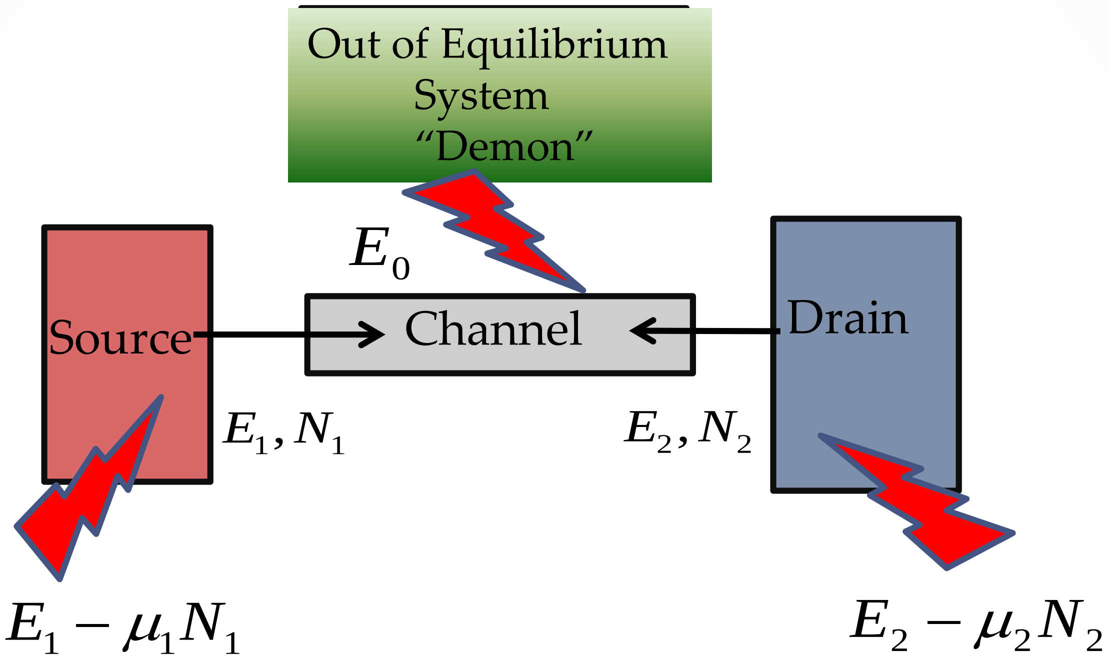
Information driven quantum dot thermal machines



Bhaskaran Muralidharan
Dept. of Electrical Engineering,
Indian institute of technology Bombay

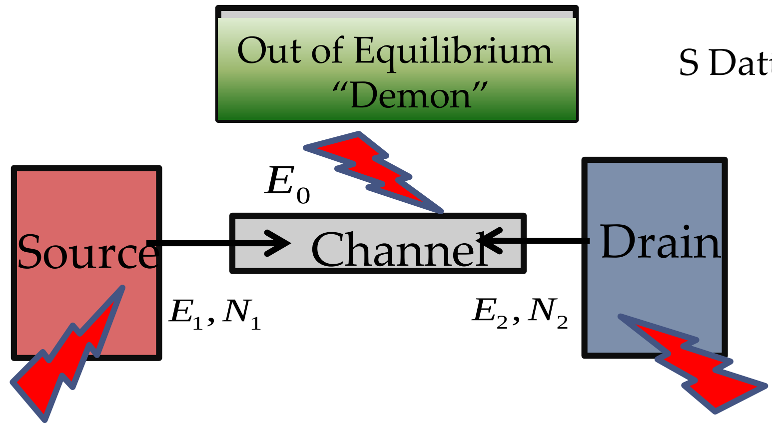
SEMINAR TALK

ICTS workshop on Open Quantum Systems

21/07/2017

Outline

- Fundamentals and Set ups
- Quantum dot heat engines

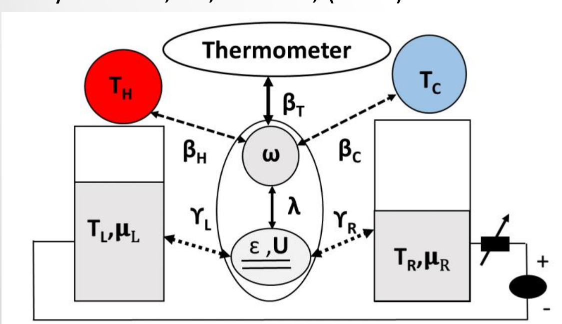


S Datta, ArXiv (2007)

$E_1 - \mu_1 N_1$ $E_2 - \mu_2 N_2$

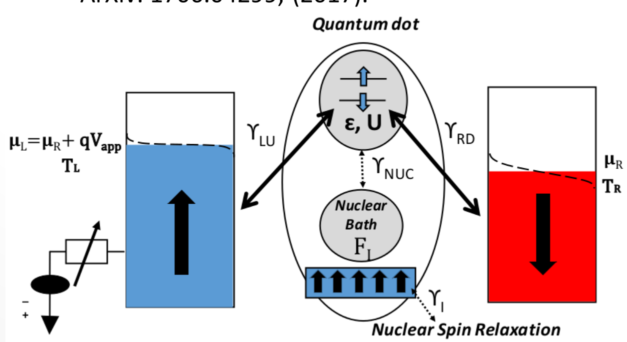
Non-equilibrium Phonons

B. De and B. Muralidharan,
Phys. Rev. B, 94, 165416, (2016).



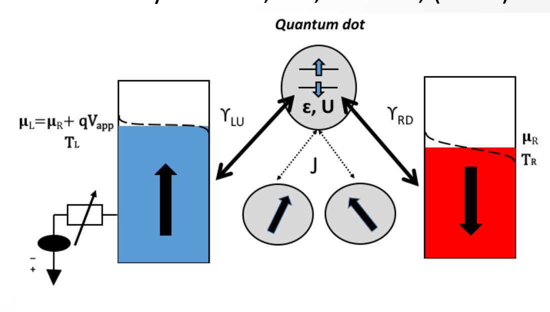
Classical Information driving

A. Shah, S. Vinjanampathy and B. Muralidharan,
ArXiv: 1706.04299, (2017).

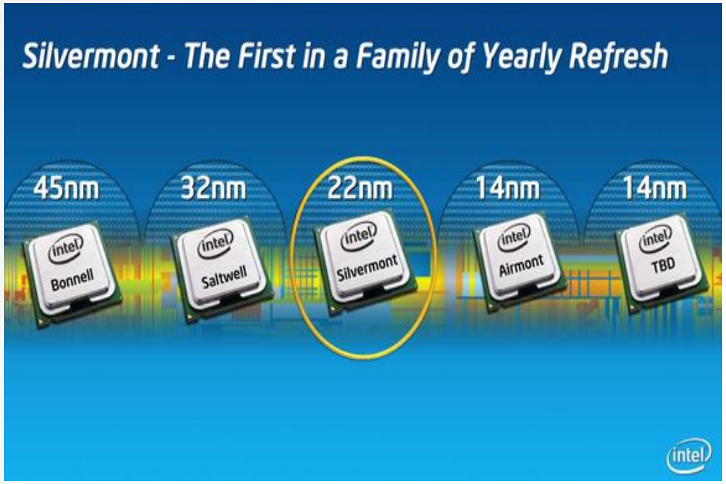


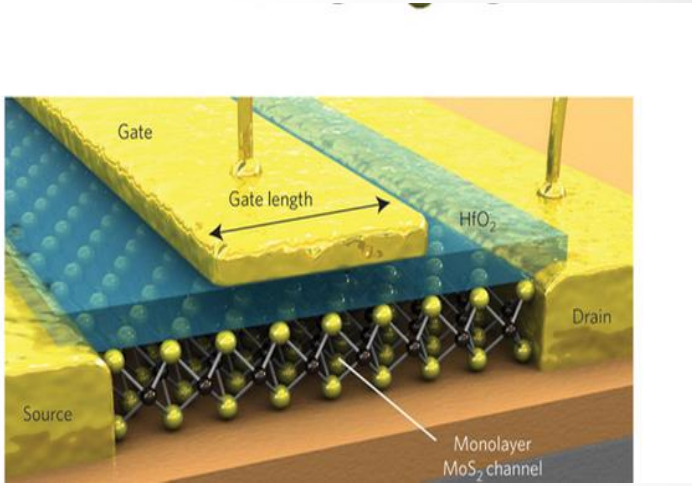
Concurrence Engine

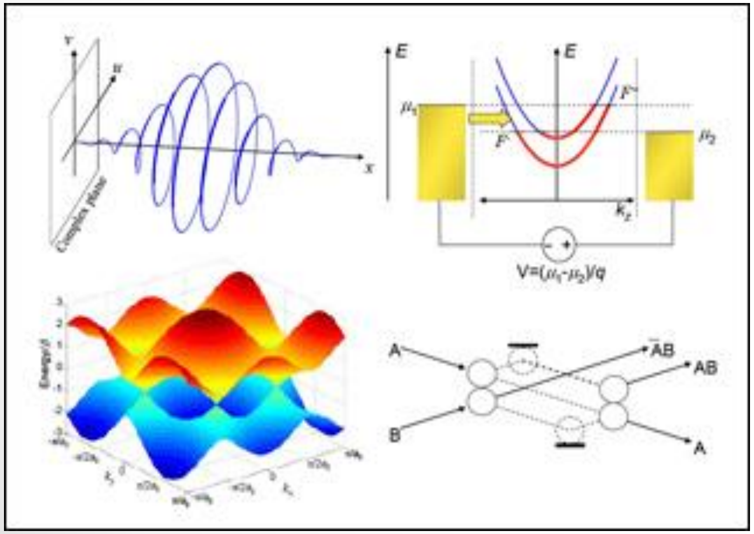
B. Muralidharan and M. Grifoni,
Phys. Rev. B, 88, 045402, (2013).

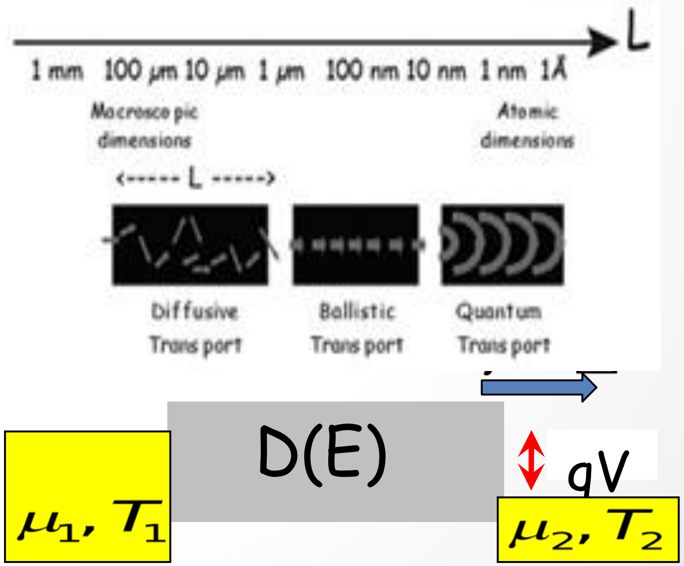


Central Theme of quantum transport: currents at the atomic level

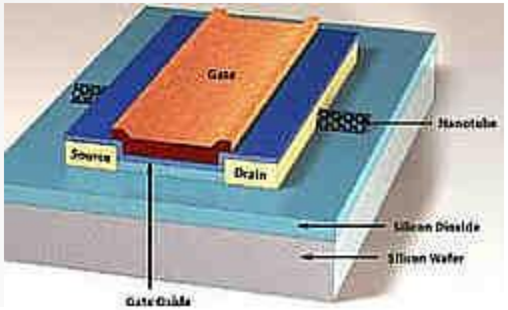


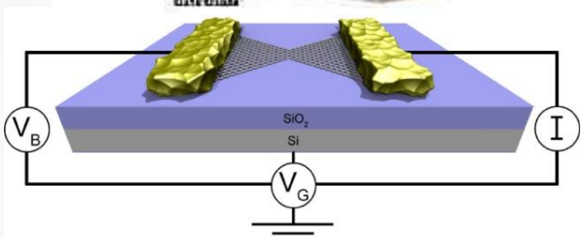


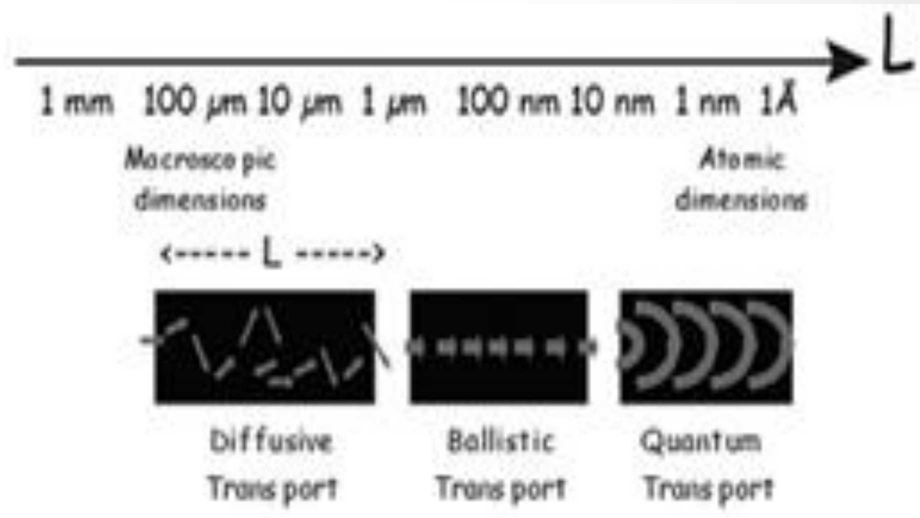


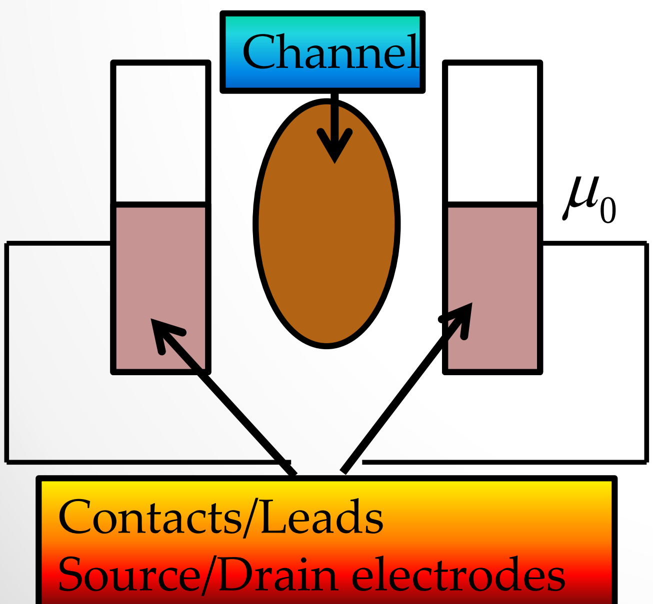


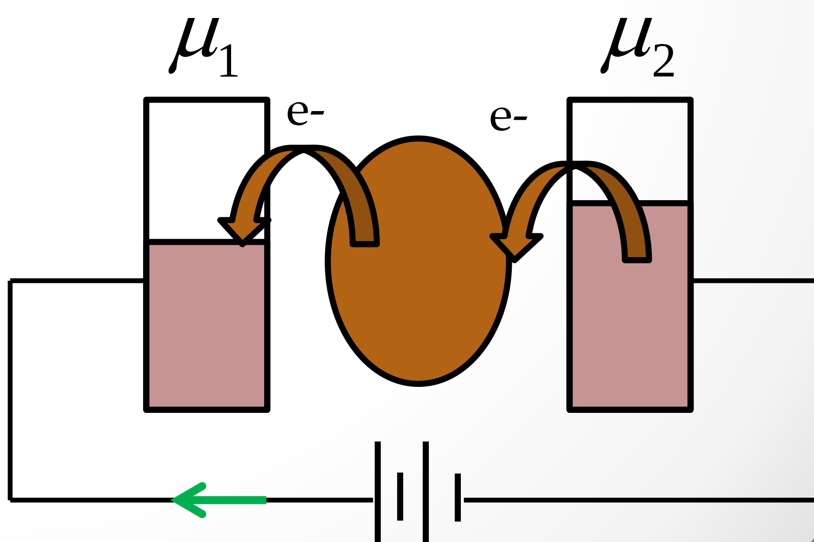
Nano-Devices



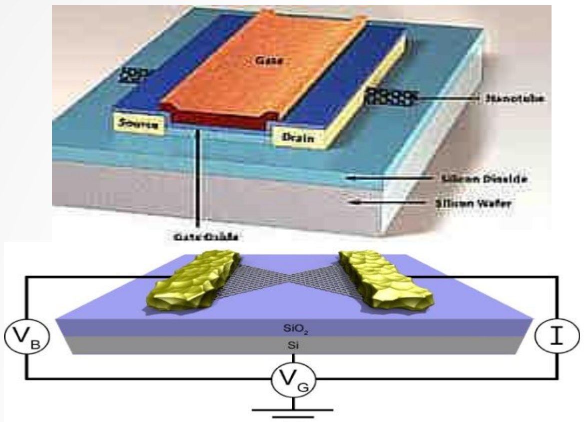




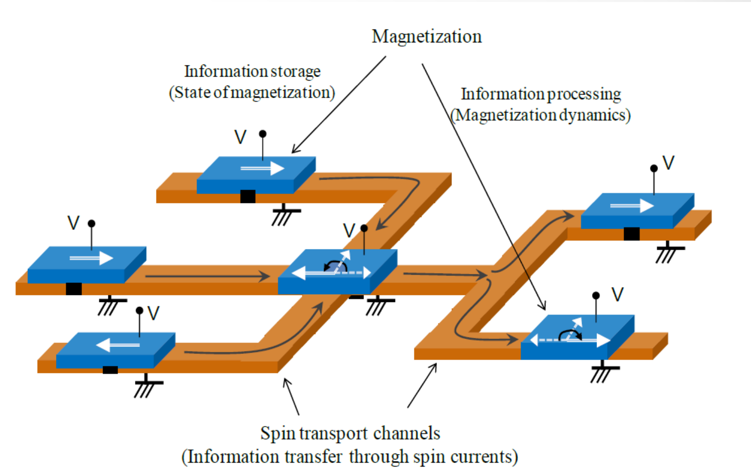




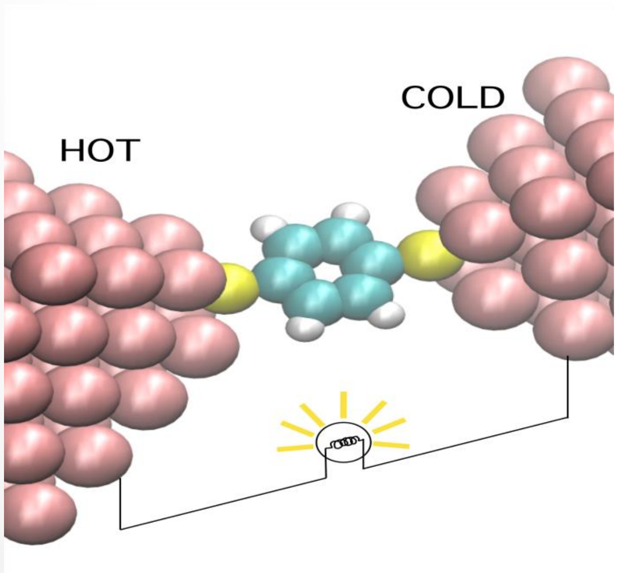
Focus Areas



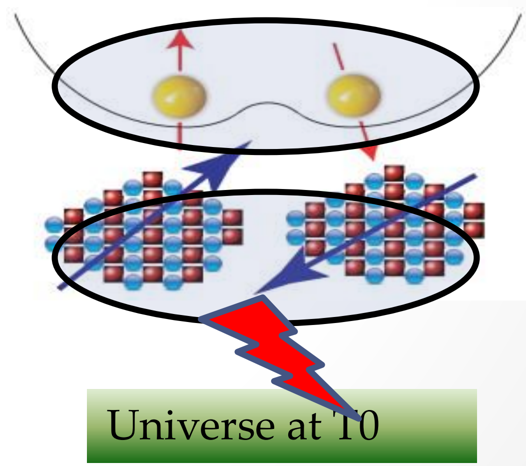
Charge based logic and memories



Spin based logic and memories

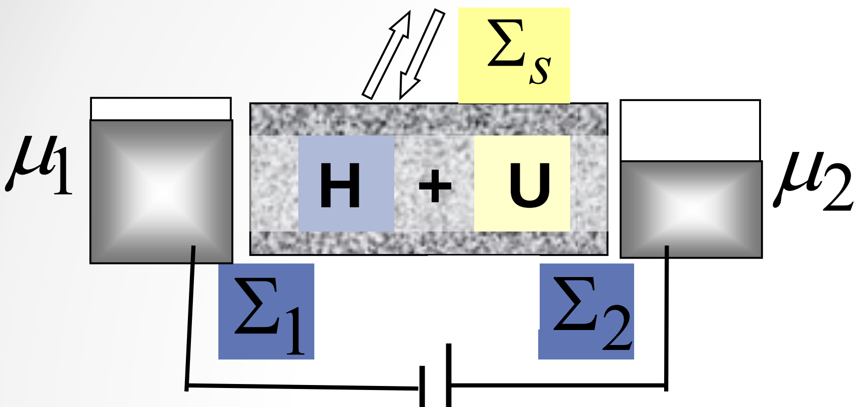


Nanoscale energy transfer



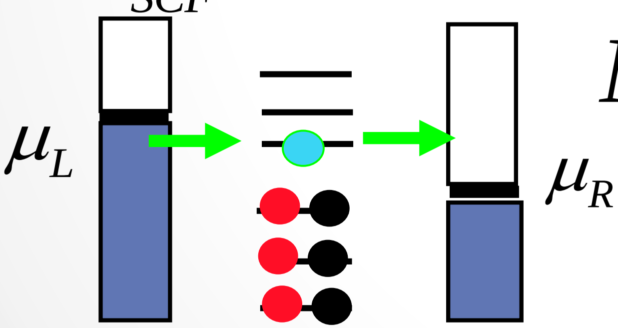
Single spin manipulation for quantum information processing

Regimes of transport



U-> Self Consistent field

$$U_{SCF} = U < n >$$

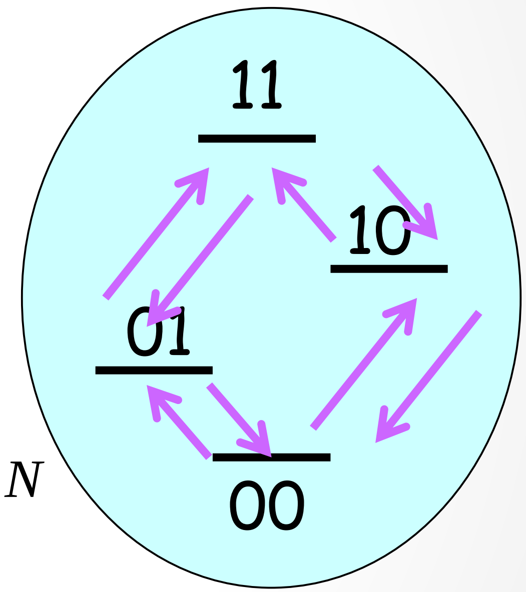


$$N \times N$$

SCF Regime

Works for $\Gamma \geq U$

2^N many electron levels



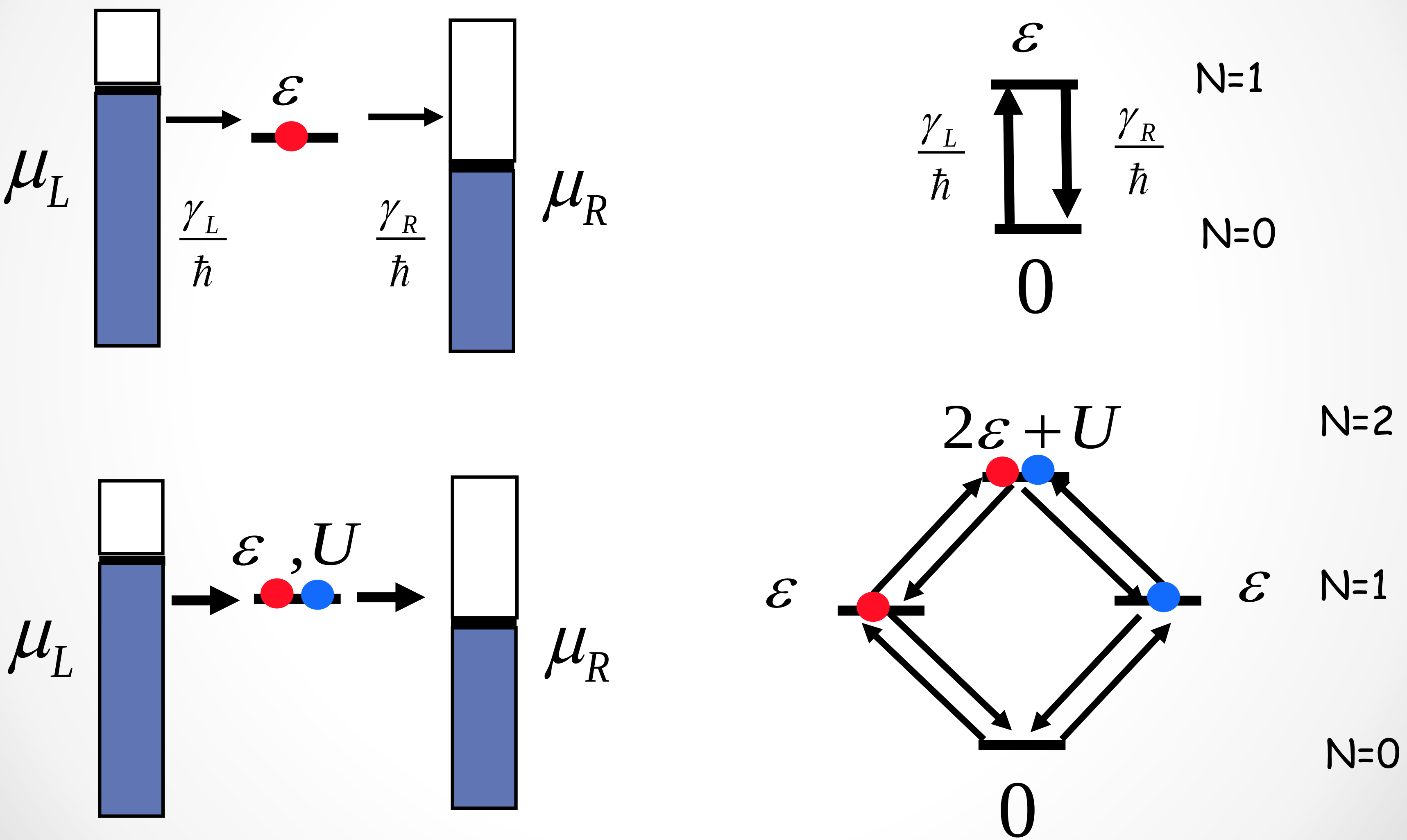
$$2^N \times 2^N$$

Fock space approach
CWJ Beenakker (1991)

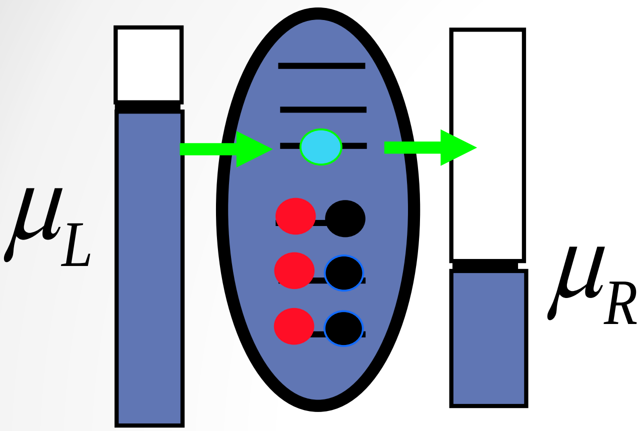
CB Regime

Works for $\Gamma << U$

Fock space picture

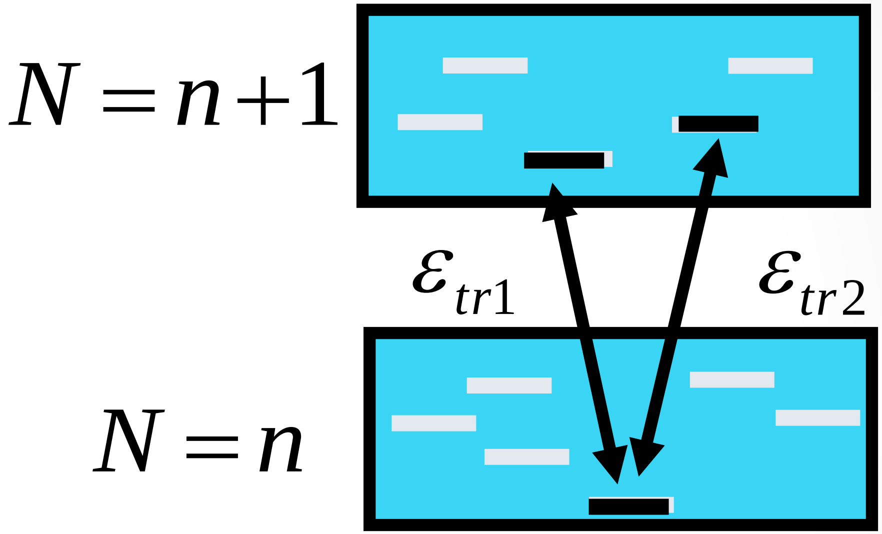


Generalized Viewpoint



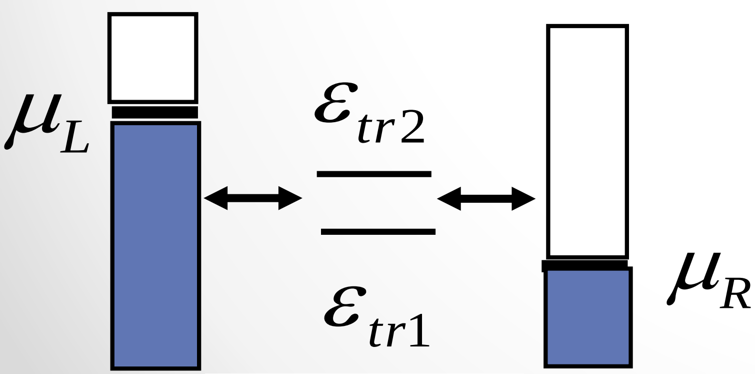
$N \times N$

$N = n$



$\{P_i\}$

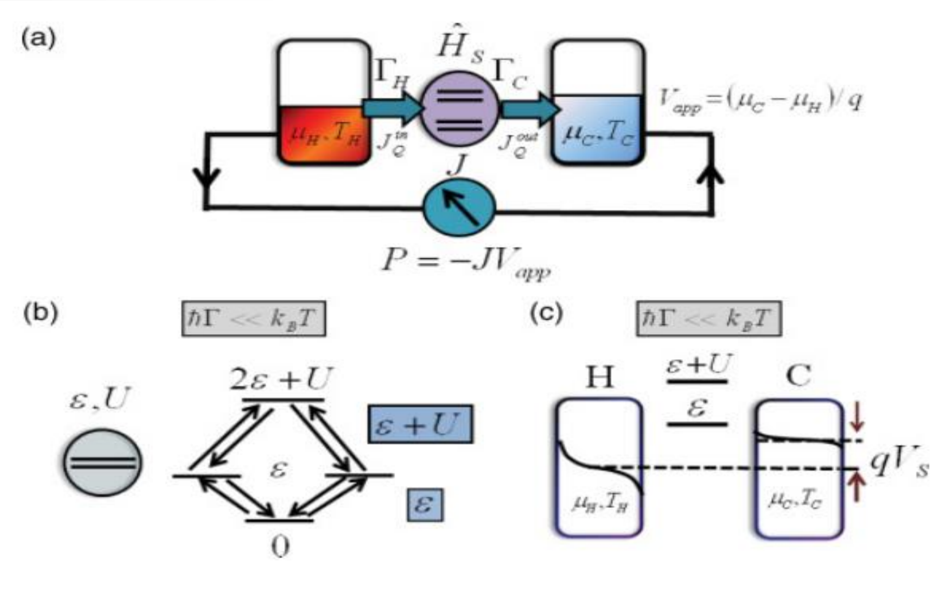
$2^N \times 2^N$

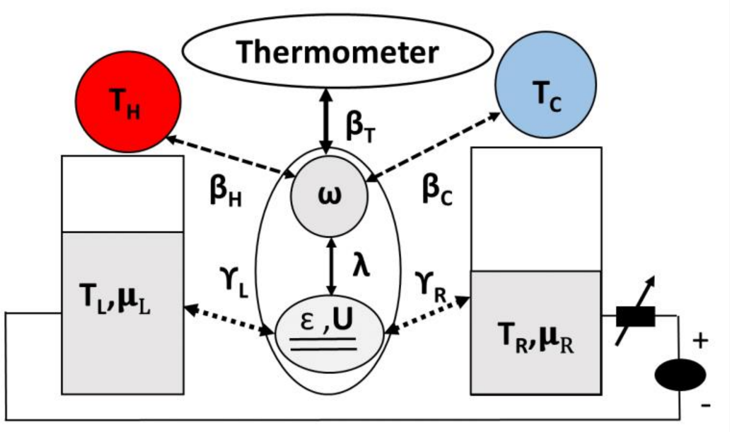


Given a bias point a set of Fock states
are probabilistically distributed!

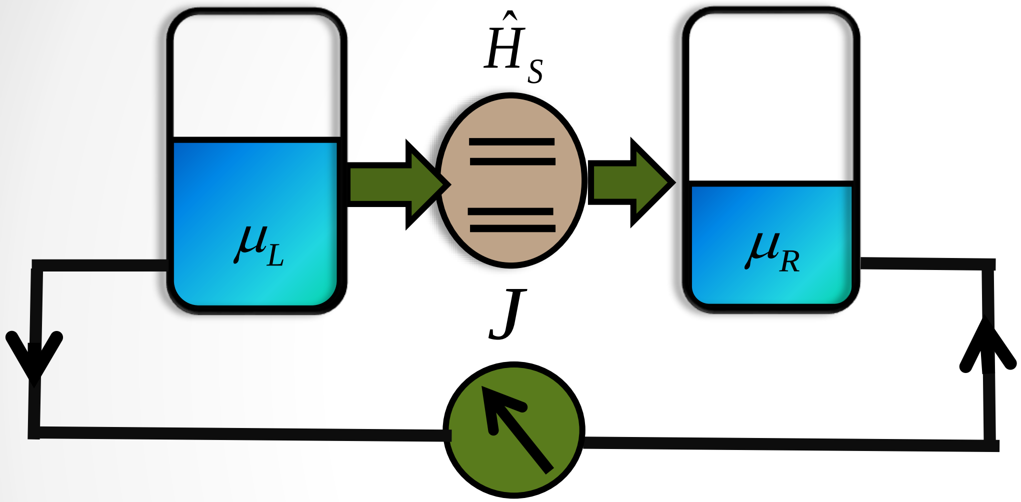
These may be viewed as transition
Energies in the one-particle picture

Part II: Quantum Dot Heat Engines

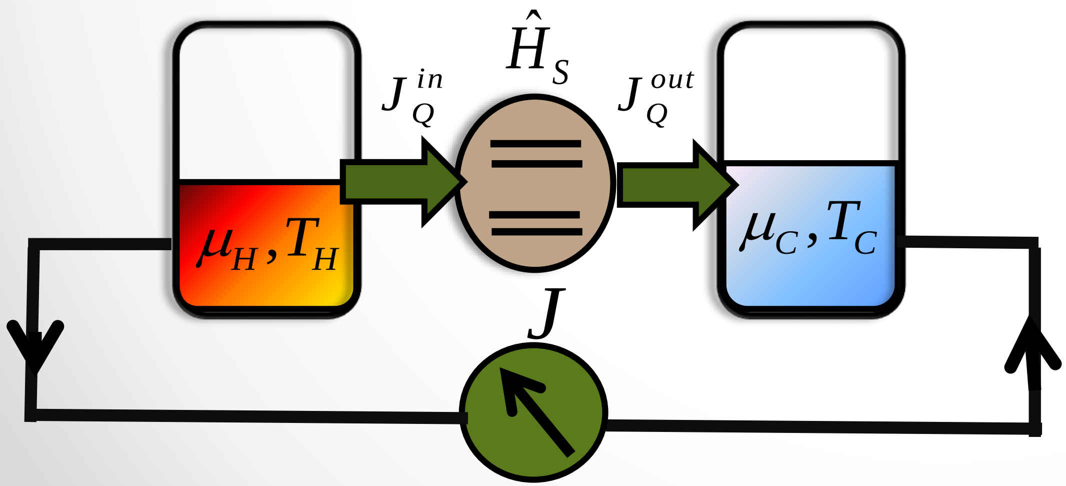




PRELIMINARIES



Electronic transport in the Presence of electrochemical Potential gradients.

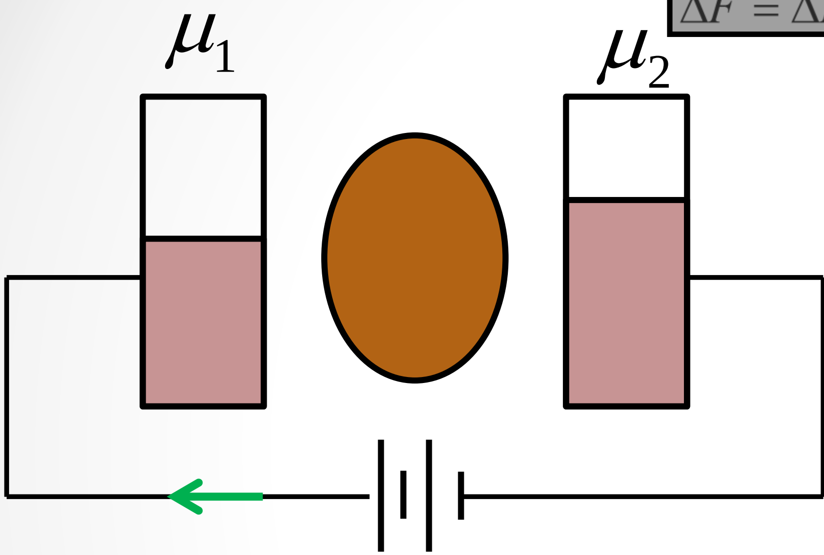


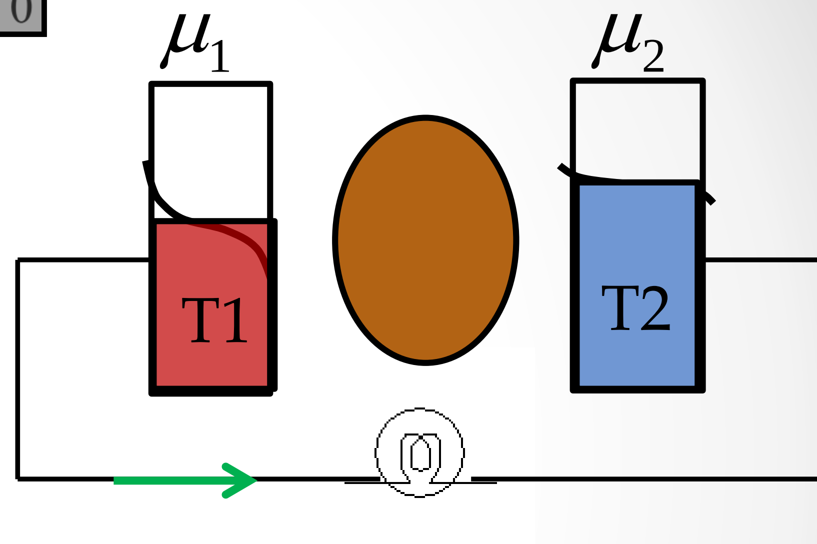
Thermoelectric transport in the presence of electrochemical potential and temperature gradients.

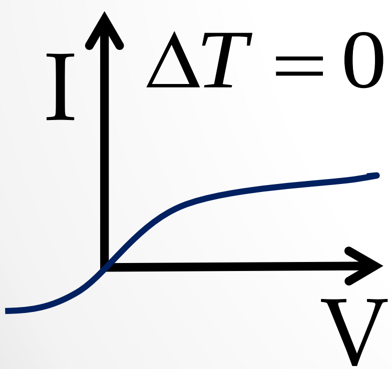
ENERGY CONVERSION!!

Nanoscale Devices/Heat Engines?

$$\Delta S_{tot} \geq 0$$
$$\Delta F = \Delta E - T\Delta S \leq 0$$

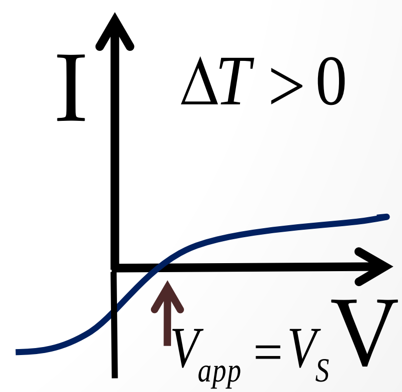






$$E = TS - pV + \mu N + HM$$
$$F = E - TS$$
$$\dot{S} = \sum_n F_n J_n$$
$$\dot{S} = \Delta(\frac{1}{T})J_Q - \frac{1}{T}V_{app}J - \frac{1}{T}\Delta\mu_s J_M$$

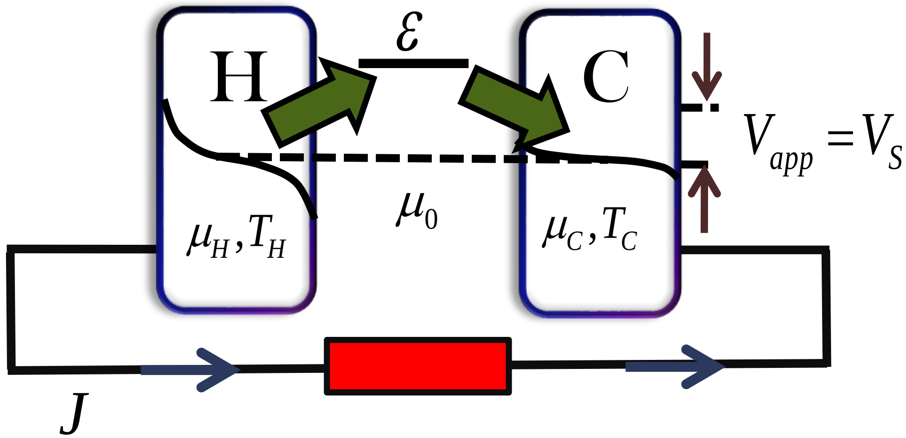
Onsager-Callen theory



$$\mu_1 N_1 + \mu_2 N_2 \geq 0$$
$$N_1 = -N_2$$

$$\frac{E - \mu_1}{T_1} \geq \frac{E - \mu_2}{T_2}$$
$$N_2 = -N_1$$

Thermodynamics of a resonant state

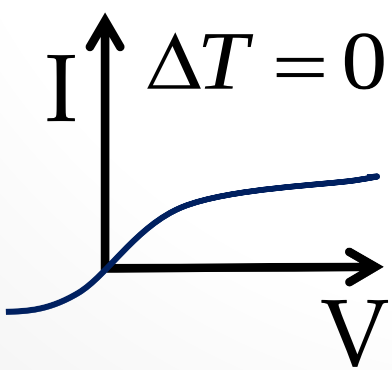


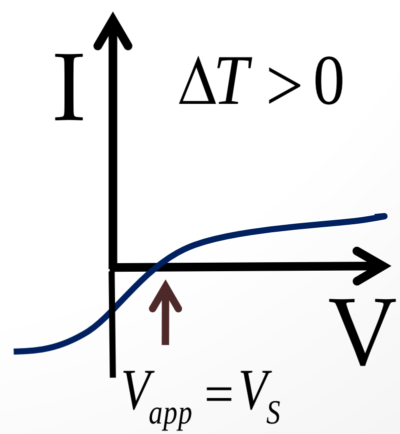
$$E = TS - pV + \mu N + HM$$

$$\dot{S} = \sum_n F_n J_n$$

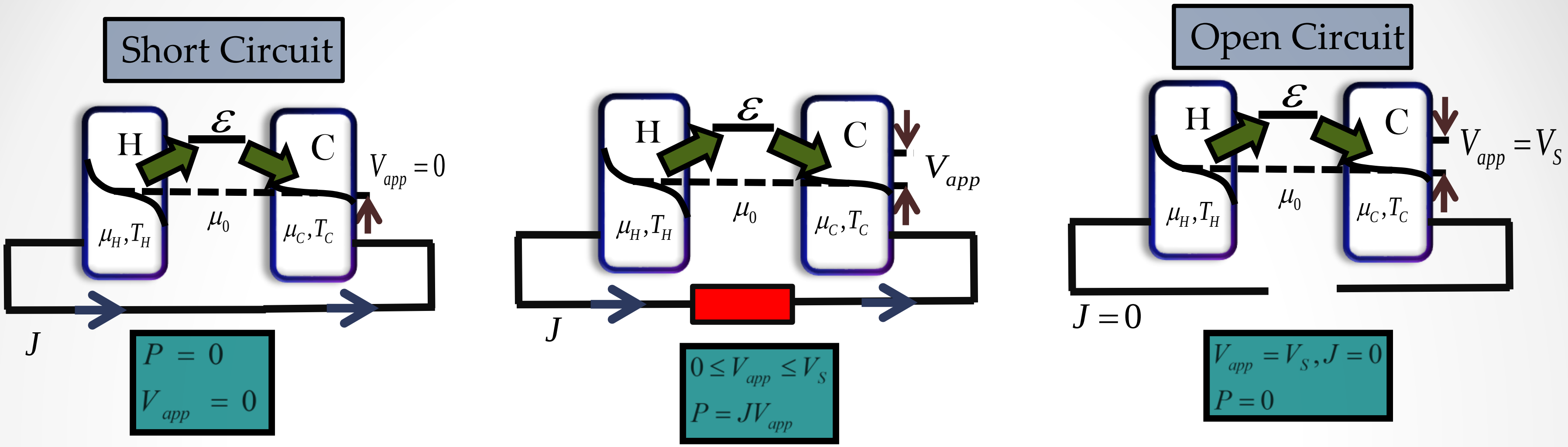
$$\dot{S} = \Delta\left(\frac{1}{T}\right) J_Q - \frac{1}{T} V_{app} J - \frac{1}{T} \Delta\mu_s J_M$$

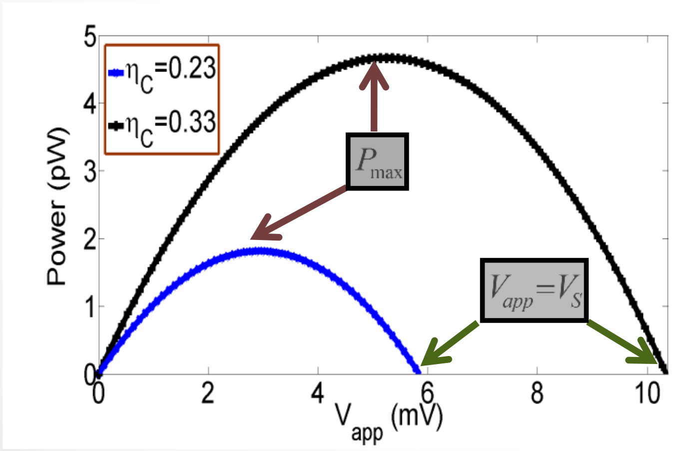
Callen-Onsager theory

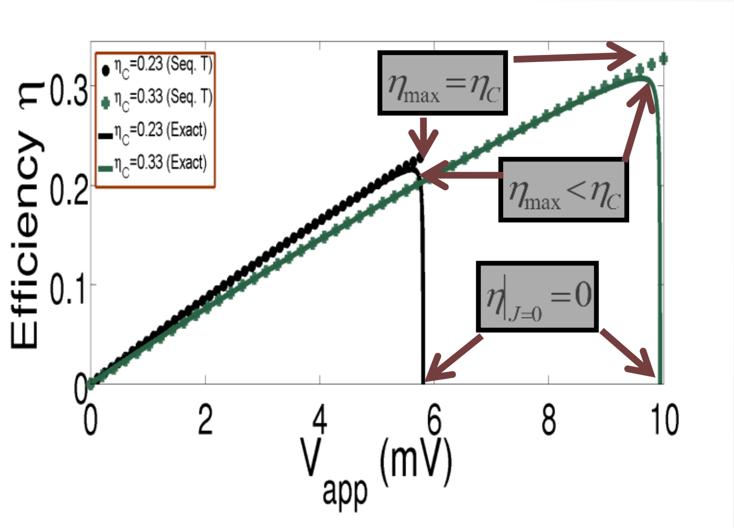




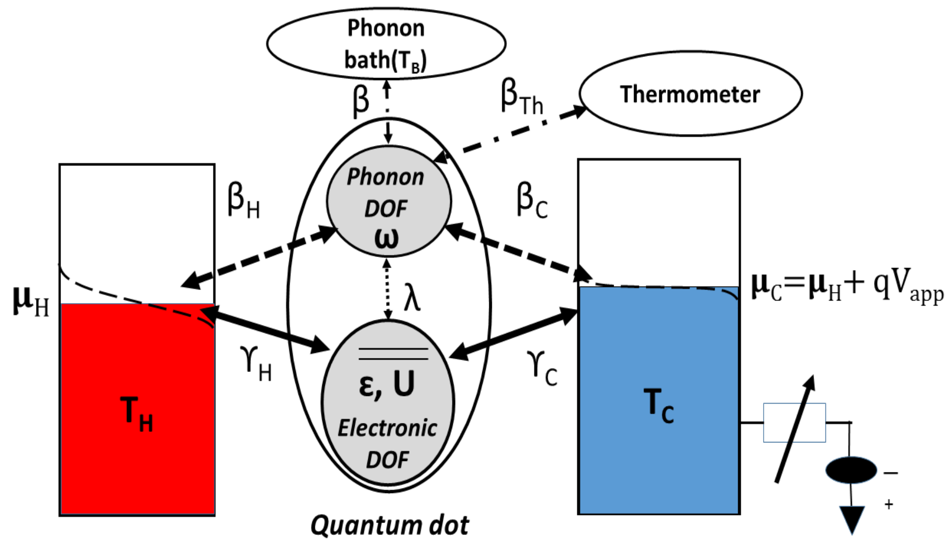
Thermoelectric operation: Power







Role of Non-equilibrium phonons



The system Hamiltonian

$$\hat{H}_D = (\sum_{\sigma} \epsilon_\sigma \hat{n}_\sigma + U\hat{n}_\uparrow \hat{n}_\downarrow) + \hbar\omega_\nu \hat{n}_\nu + \sum_{\sigma} \lambda_\nu \hbar\omega_\nu \hat{n}_\sigma (\hat{b}_\nu^\dagger + \hat{b}_\nu),$$

The dot Hamiltonian

$$\hat{H}_{CD} = \sum_{k\sigma',\sigma} \tau^{el}_{\alpha k\sigma'\sigma} \hat{c}^\dagger_{\alpha k\sigma'} \hat{d}_\sigma + h.c + \sum_{\nu,p} \tau^{ph}_{\alpha p\nu} (\hat{a}^\dagger_{\alpha p} + \hat{a}_{\alpha p})(\hat{b}^\dagger_\nu + \hat{b}_\nu)$$

The Contact-dot tunneling Hamiltonian

$$\hat{H}_C = \sum_{\alpha\in H,C} \sum_{k\sigma'} \epsilon_{\alpha k\sigma'} \hat{n}_{\alpha k\sigma'} + \sum_{\alpha\in H,C} \sum_{p} \hbar\omega_{\alpha p} \hat{n}_{\alpha p}$$

The contact Hamiltonian

$$\hat{H}_{BD} = \sum_{\nu,t} \tau^{ph}_{t\nu} (\hat{B}^\dagger_t + \hat{B}_t)(\hat{b}^\dagger_\nu + \hat{b}_\nu)$$

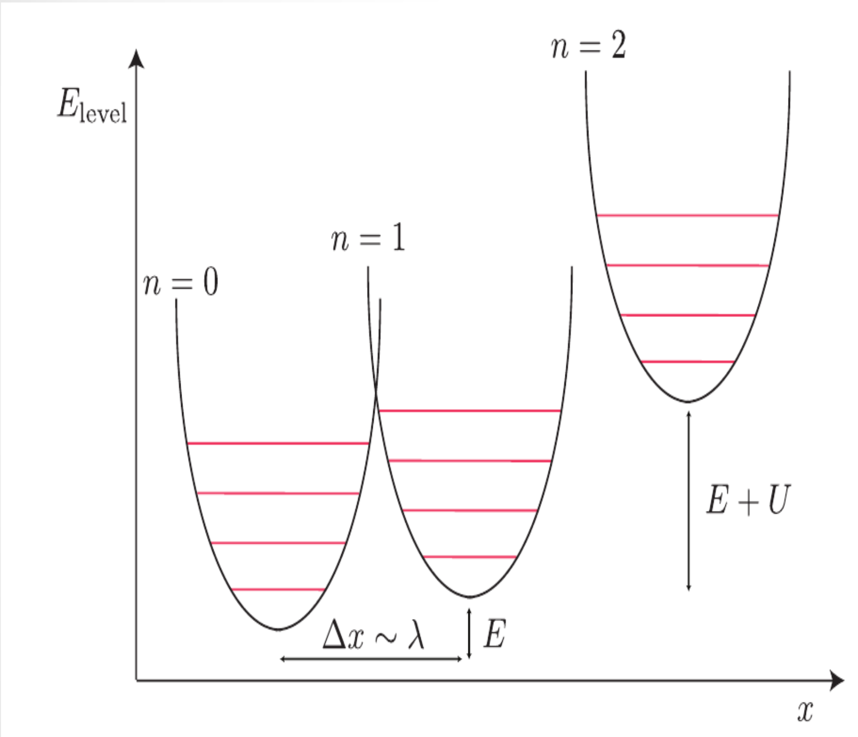
The Bath-dot phonon transition Hamiltonian

$$\hat{H}_B = \sum_{t} \hbar\omega_t \hat{B}^\dagger_t \hat{B}_t$$

The Bath Hamiltonian

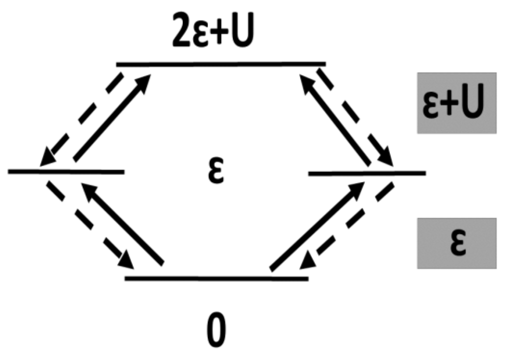
$$\hat{H} = \hat{H}_D + \hat{H}_C + \hat{H}_B + \hat{H}_{CD} + \hat{H}_{BD}$$

The Lang-Firsov transformation

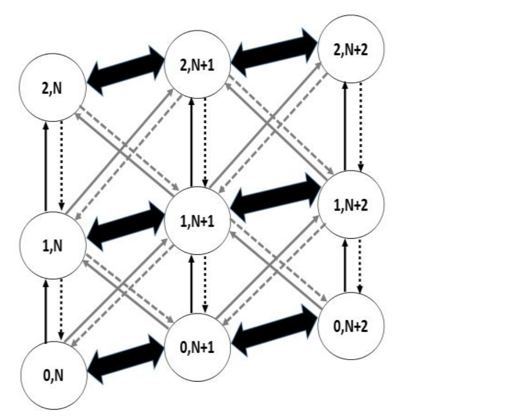


$$\tilde{\epsilon}_\sigma = \epsilon_\sigma - (\lambda^2 \hbar\omega_\nu),$$

$$\tilde{U} = U - (2\lambda^2 \hbar\omega_\nu).$$

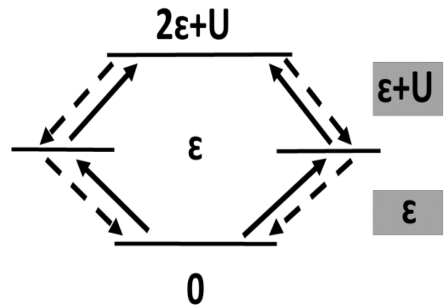


Electron Fock space



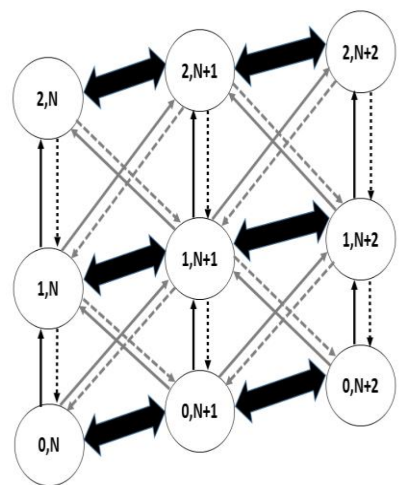
Electron-phonon Fock space

Formulation



$$R^{el}_{(n,q)\to(n+1,q')} = \sum_{\alpha\in H,C} \gamma_\alpha |\langle n,q|\hat{\tilde{d}}_\sigma|n+1,q'\rangle|^2 \times f_\alpha\left(\frac{E_{(n+1,q')}-E_{(n,q)}-\mu_\alpha}{k_B T_\alpha}\right)$$

Electron tunneling from contact to dot



$$R^{el}_{(n,q)\to(n-1,q')} = \sum_{\alpha\in H,C} \gamma_\alpha |\langle n,q|\hat{\tilde{d}}^\dagger_\sigma|n-1,q'\rangle|^2 \times\left[1-f_\alpha\left(\frac{E_{(n,q)}-E_{(n-1,q')}-\mu_\alpha}{k_B T_\alpha}\right)\right]$$

Electron tunneling from dot to contact

$$\gamma_\alpha = \sum_{k\sigma'} \frac{2\pi}{\hbar}|\tilde{\tau}^{el}_{\alpha k\sigma'}|^2\delta(E-\epsilon_{\alpha k\sigma'})$$

$$R^{ph}_{(n,q)\to(n,q+1)} = \sum_{r'\in H,C,B} \beta_{r'}(q+1)exp(-\frac{\hbar\omega_r}{k_B T_{r'}})$$

$$\beta_{r'} = \sum_r \frac{2\pi}{\hbar}|\tilde{\tau}^{ph}_{r\nu}|^2\delta(\omega-\omega_r)$$

$$R^{ph}_{(n,q)\to(n,q-1)} = \sum_{r'\in H,C,B} \beta_{r'}(q+1).$$

Bath assisted phonon absorption

Bath assisted phonon relaxation

Currents

$$\frac{dP_{(n,q)}}{dt} = \sum_{k'=0}^{N_q'-1} \Big[R^{el}_{(n\pm1,q')\to(n,q)} P_{(n\pm1,q')} - R^{el}_{(n,q)\to(n\pm1,q')} P_{(n,q)} \Big] + \Big[R^{ph}_{(n,q\pm1)\to(n,q)} P_{(n,q\pm1)} - R^{ph}_{(n,q)\to(n,q\pm1)} P_{(n,q)} \Big].$$

Master equation

$$J^Q_{el_\alpha} = \sum_{n,q=0}^{N_e,N_p-1} \sum_{k'}^{N_p'-1} \Big[E_{(n\pm1,q')} - \mu_\alpha \Big] \times R^{el_\alpha}_{(n\pm1,q')\to(n,q)} P_{(n\pm1,q')} - \Big[E_{(N_e,N_p)} - \mu_\alpha \Big] \times R^{el_\alpha}_{(n,q)\to(n\pm1,q)} P_{(n,q)}$$

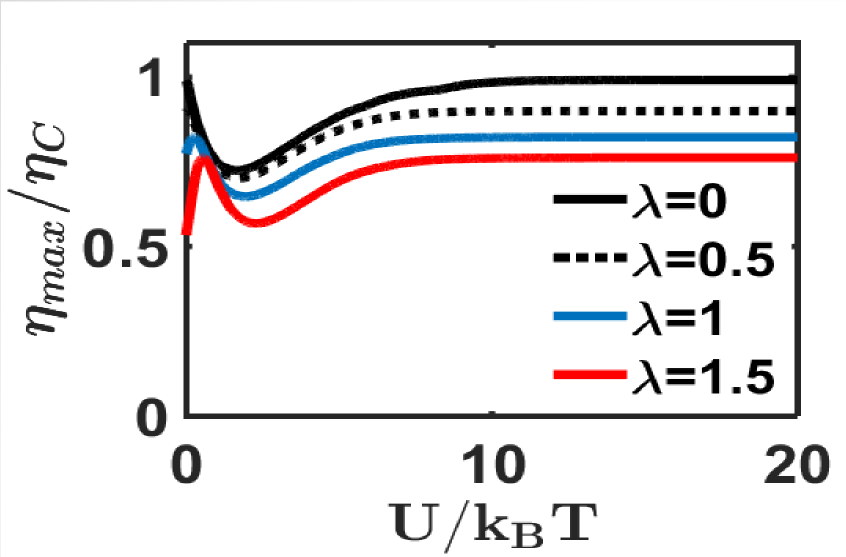
Electron heat current

$$J_\alpha = \sum_{n,q=0}^{N_e,N_p-1} \sum_{q'=0}^{N_q'-1} -q \Big[R^{el_\alpha}_{(n\pm1,q')\to(n,q)} P_{(n\pm1,q')} - R^{el_\alpha}_{(n,q)\to(n\pm1,q')} P_{(n,q)} \Big]$$

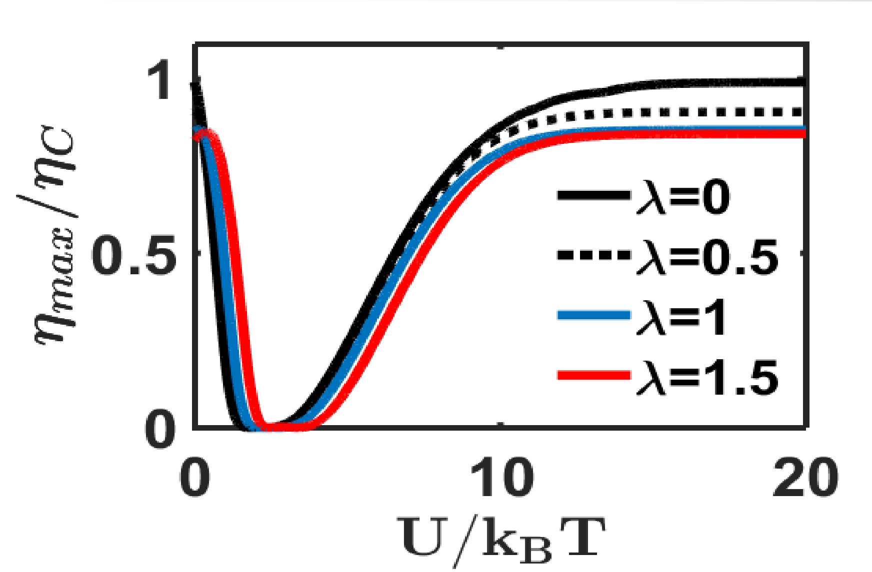
Electron charge current

$$J^Q_{ph_{r'}} = \sum_{n,q=0}^{N_e,N_p-1} \hbar\omega_r \Big[R^{ph_\alpha}_{(n,q)\to(n,q\pm1)} P_{(n,q)} - R^{ph_\alpha}_{(n,q\pm1)\to(n,q)} P_{(n,q+1)} \Big]$$

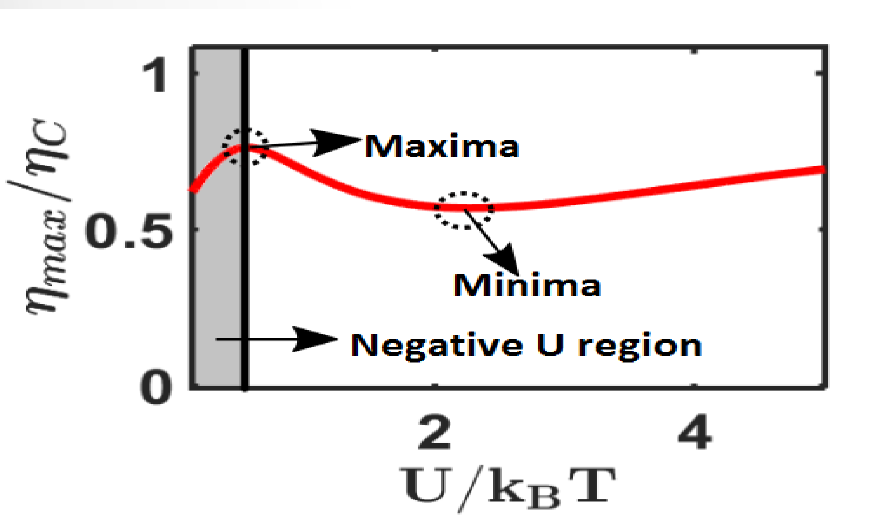
Phonon heat current



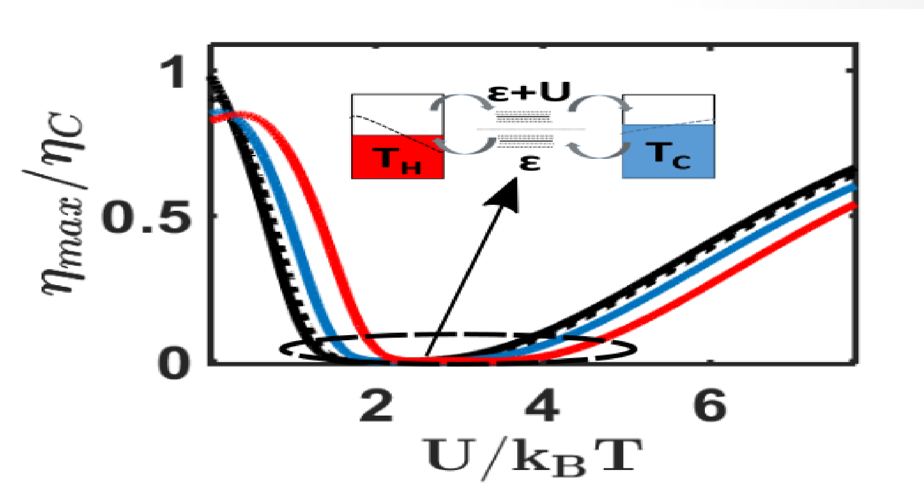
n-type quantum dot



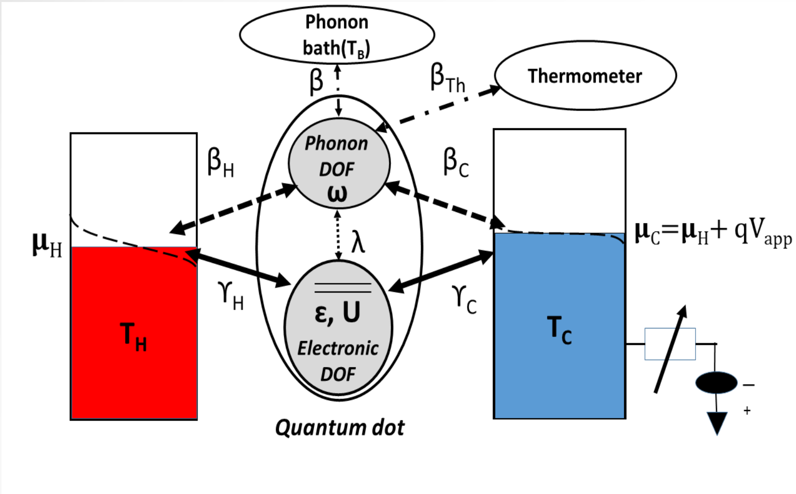
p-type quantum dot



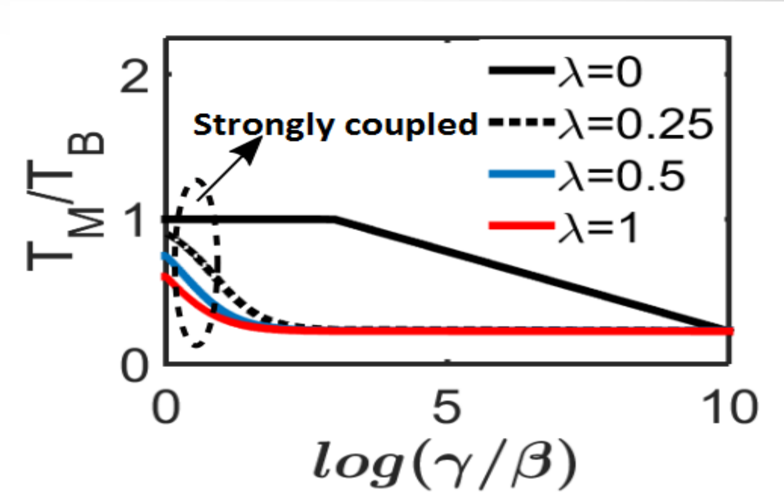
Negative U region



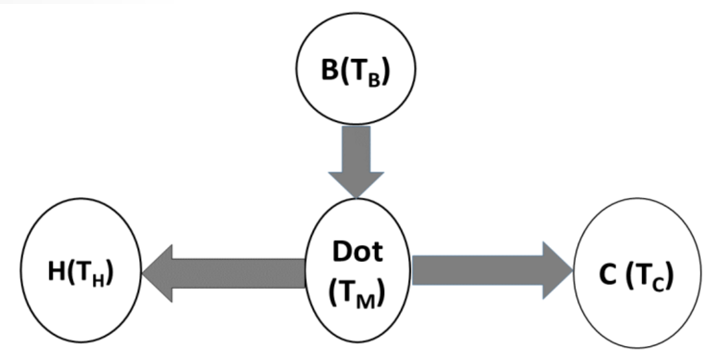
Particle-hole symmetry



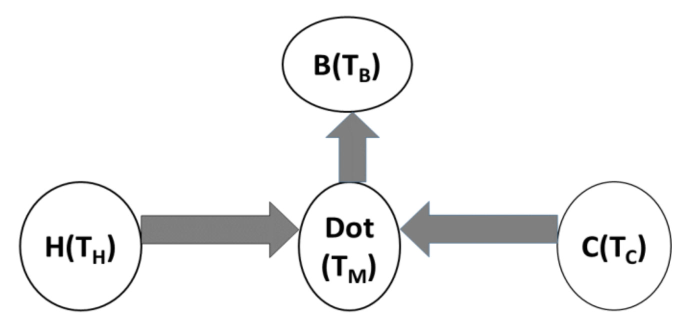
Circuit diagram of the set-up



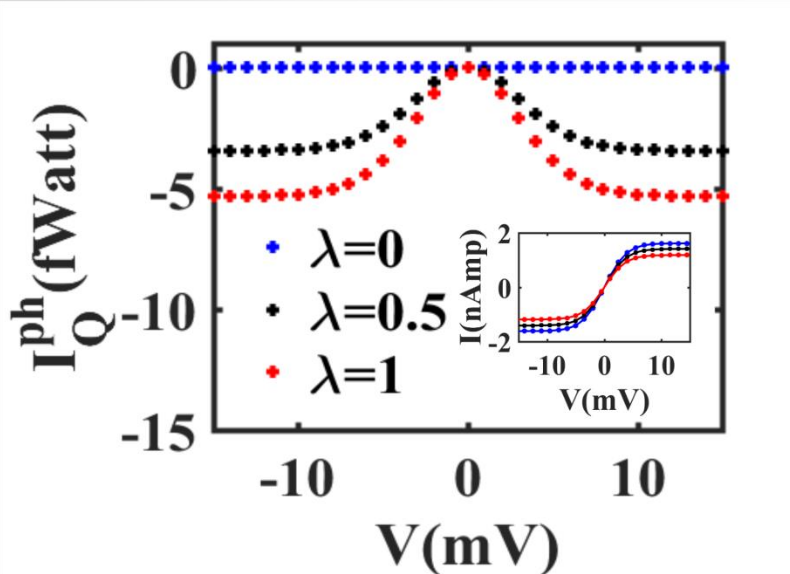
Deviation of dot temperature with interaction and bath coupling

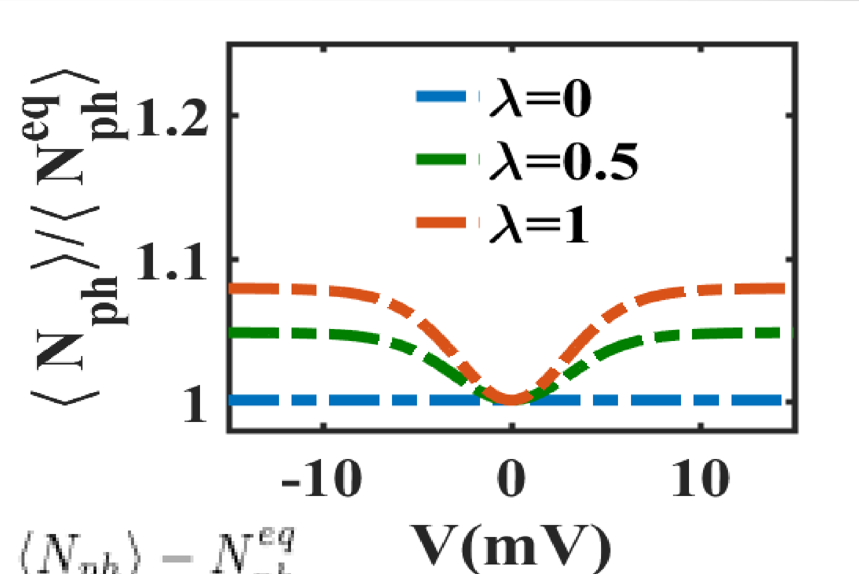


Hot phonon bath

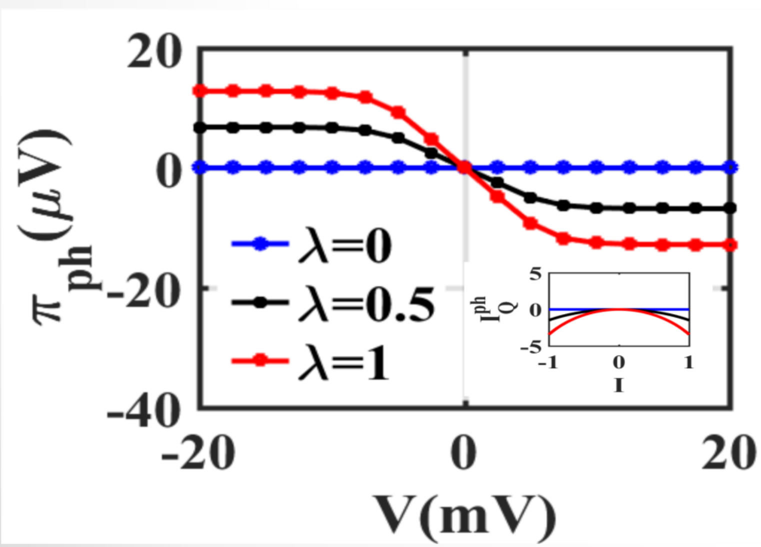


Cold phonon bath

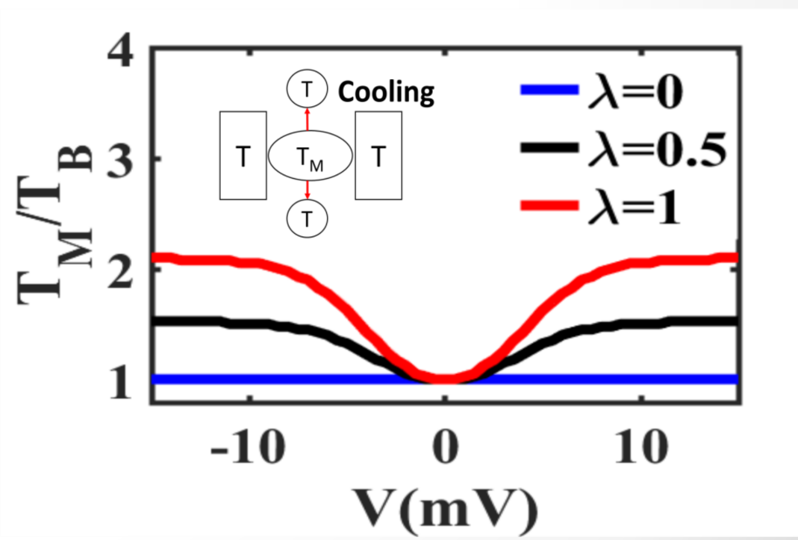




$$RE_{ph}^{\alpha_2} = \beta_{\alpha_2}\frac{\langle N_{ph}\rangle - N_{ph}^{eq}}{1+N_{ph}^{eq}}.$$

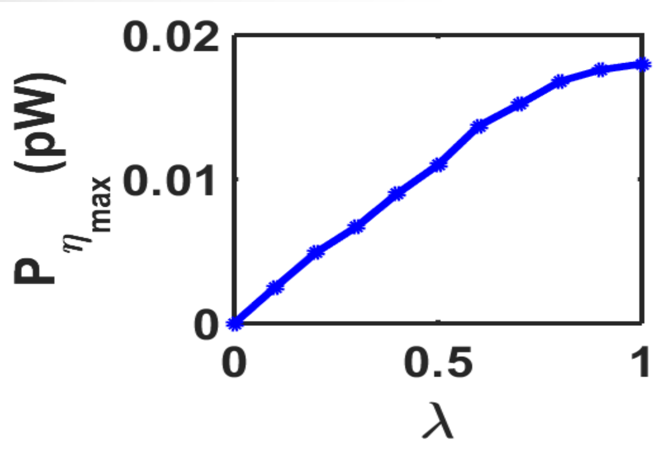


Phonon Peltier coefficient

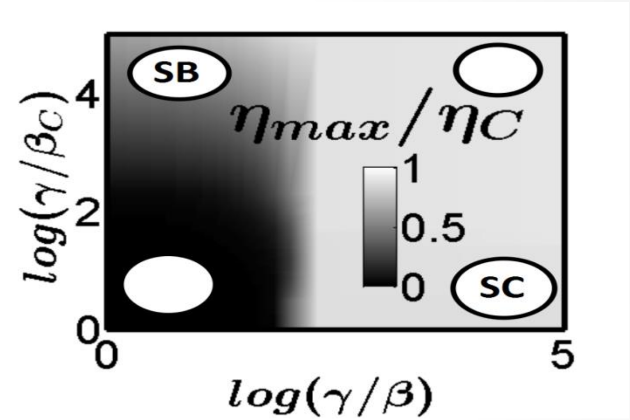


Peltier cooling

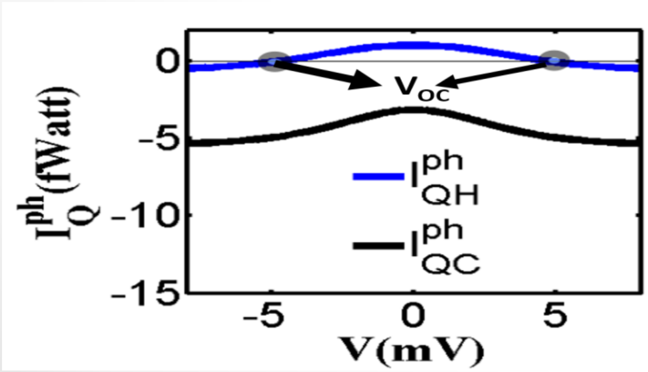
Applications



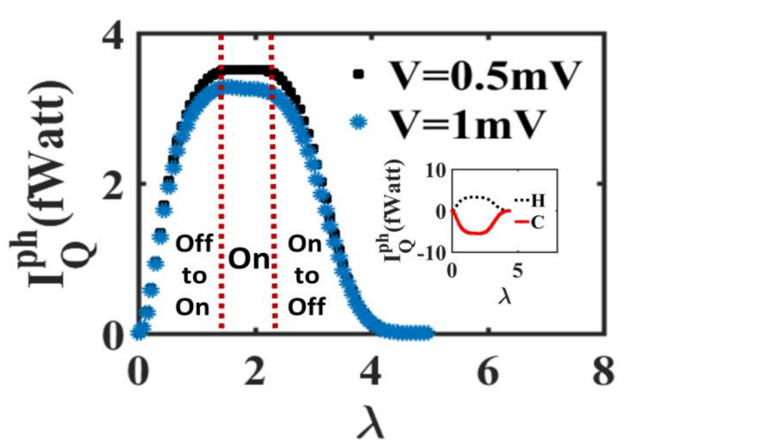
Power-efficiency trade off



Optimization of efficiency

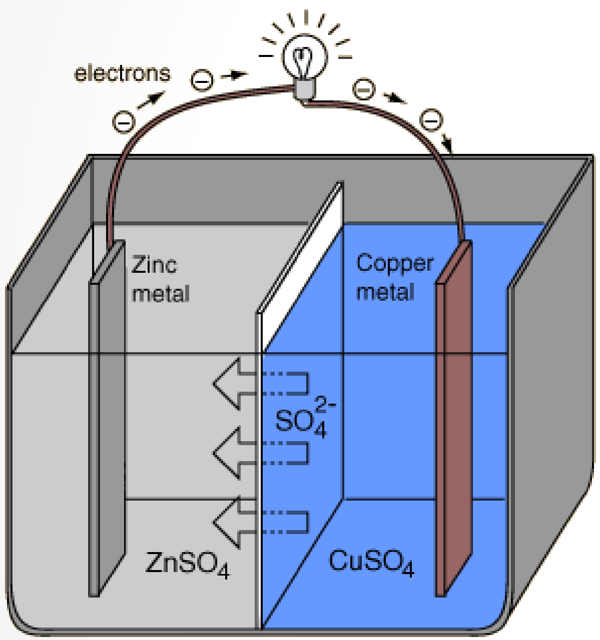


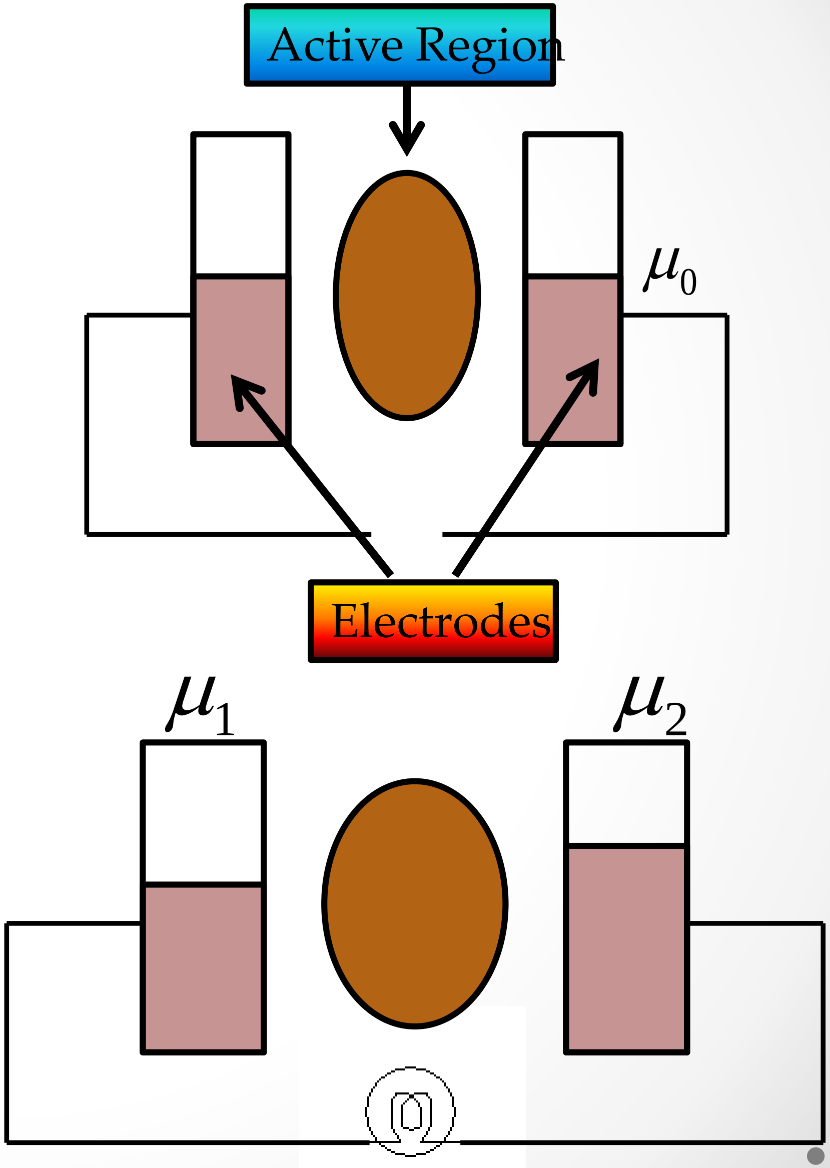
Cooling through Hot bath



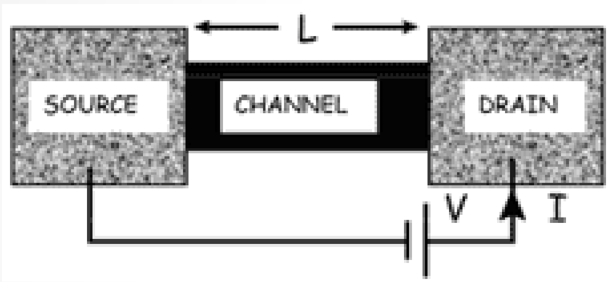
Electron induced phonon switching

Battery Operation Schematic

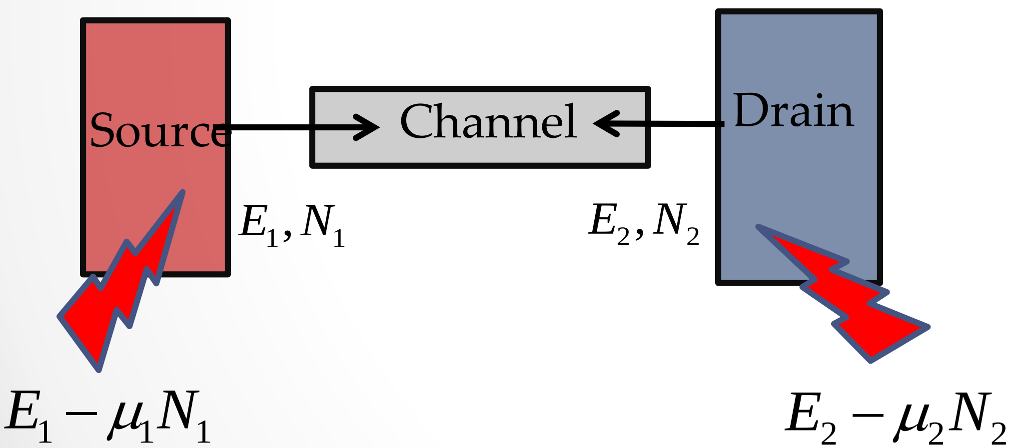




Nanoscale Devices-The energy picture



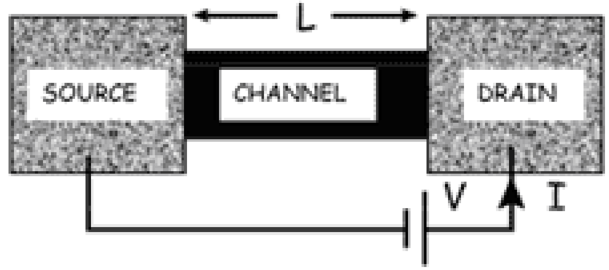
$$
\begin{aligned}
&N_1 + N_2 = 0\\
&E_1 + E_2 = 0\\
&\frac{E_1 - \mu_1 N_1}{T_1} + \frac{E_2 - \mu_2 N_2}{T_2} \le 0
\end{aligned}
$$



$$
\begin{aligned}
&\frac{E_1 - \mu_1 N_1}{T_1} + \frac{E_2 - \mu_2 N_2}{T_2} \le 0\\
&-\Delta S_1 - \Delta S_2 \le 0
\end{aligned}
$$

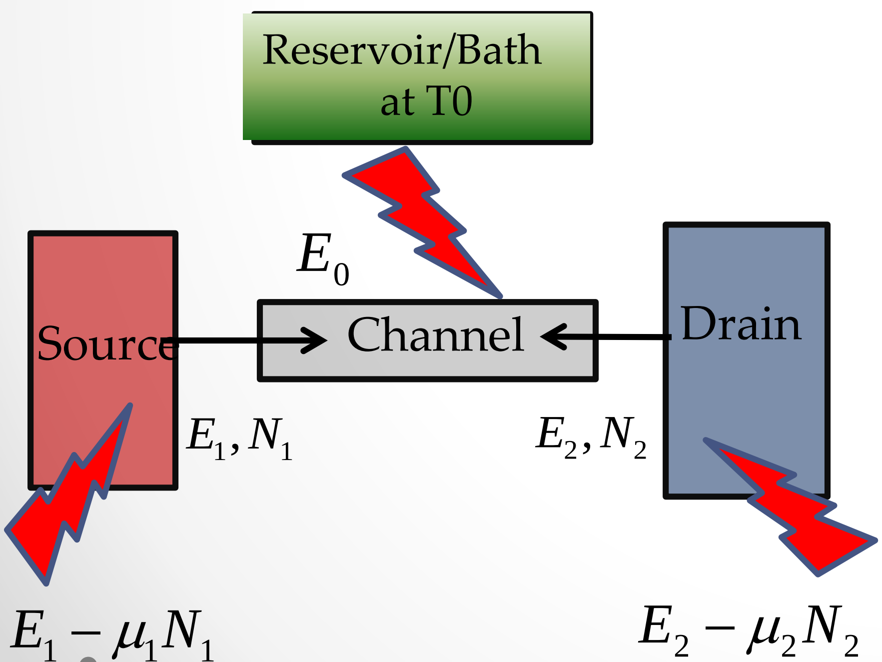
Heat Engines with demons

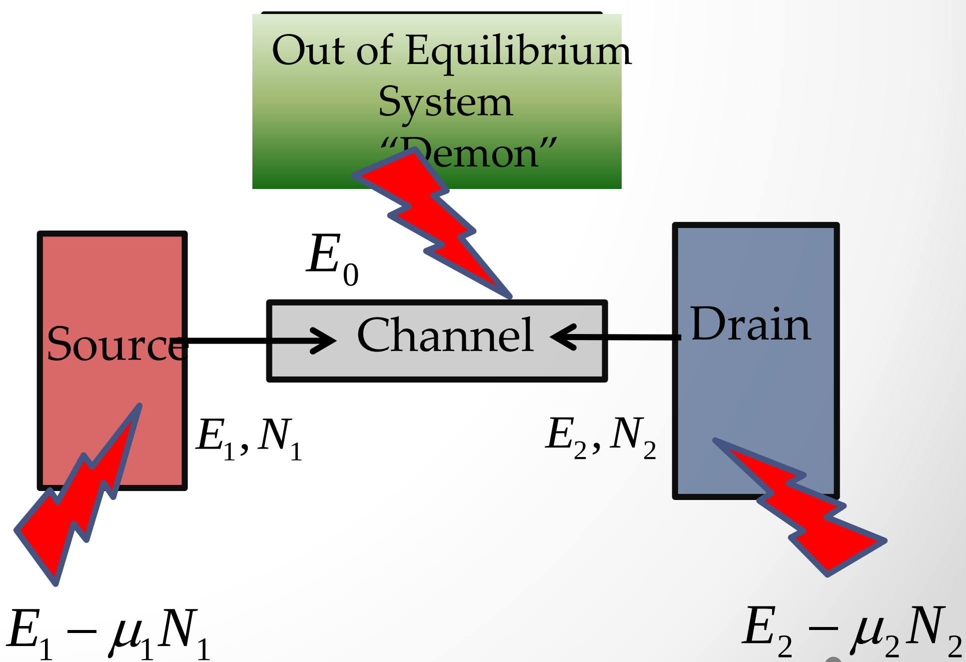
$$N_1 + N_2 = 0$$
$$E_1 + E_2 + E_0 = 0$$
$$\frac{E_1 - \mu_1 N_1}{T_1} + \frac{E_2 - \mu_2 N_2}{T_2} + \frac{E_0}{T_0} \le 0$$



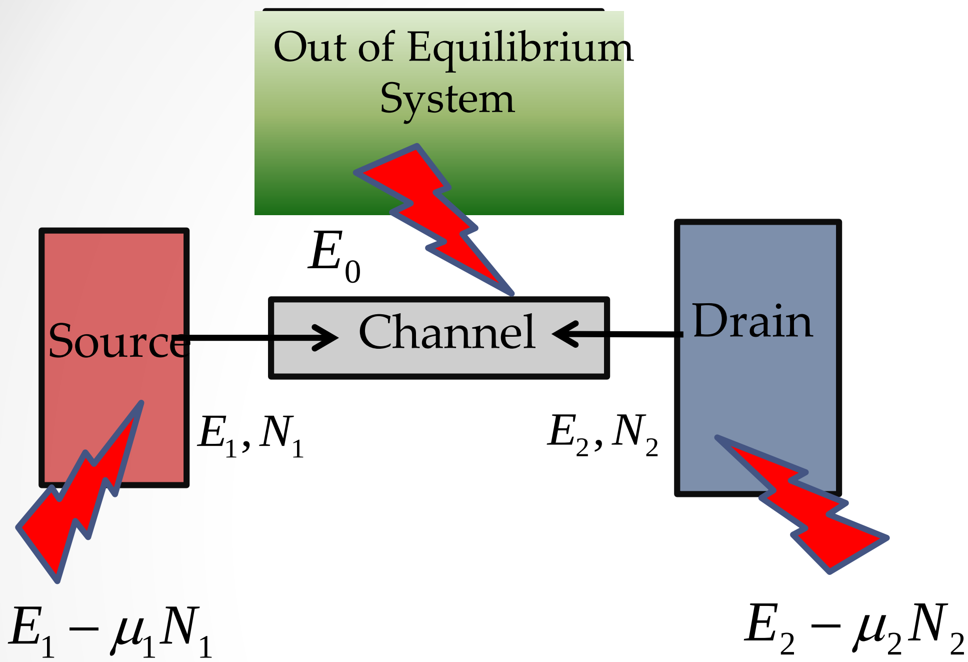
$$N_1 + N_2 = 0$$
$$E_1 + E_2 + E_0 = 0$$
$$\frac{E_1 - \mu_1 N_1}{T_1} + \frac{E_2 - \mu_2 N_2}{T_2} - \Delta S_0 \le 0$$

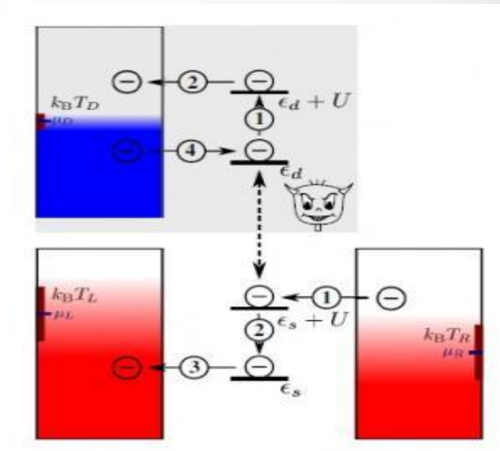
S=klnW

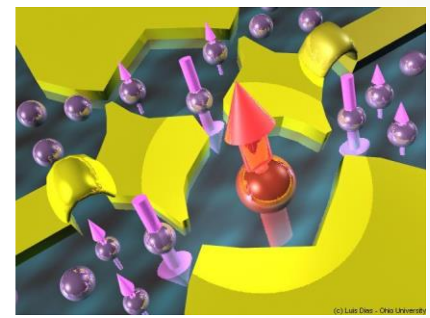


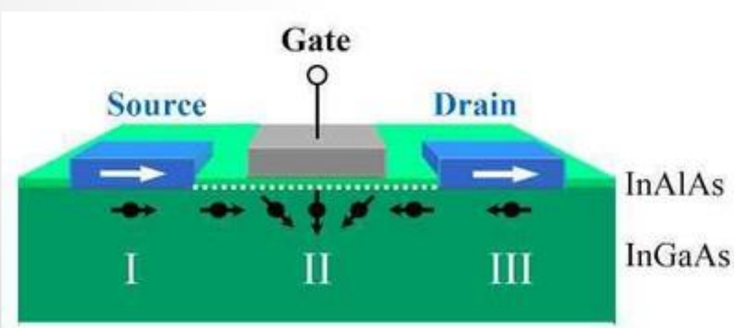


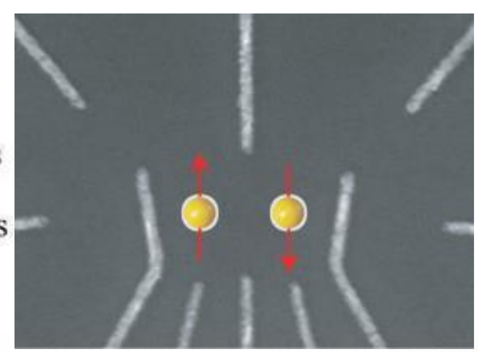
Examples of nano-device “demons”

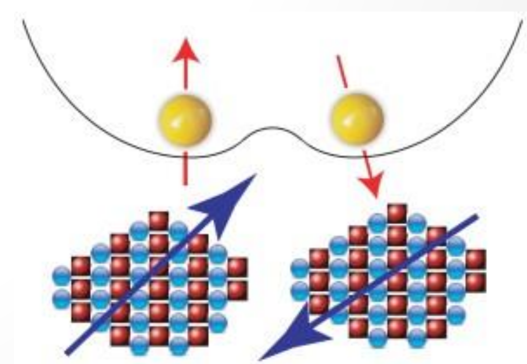




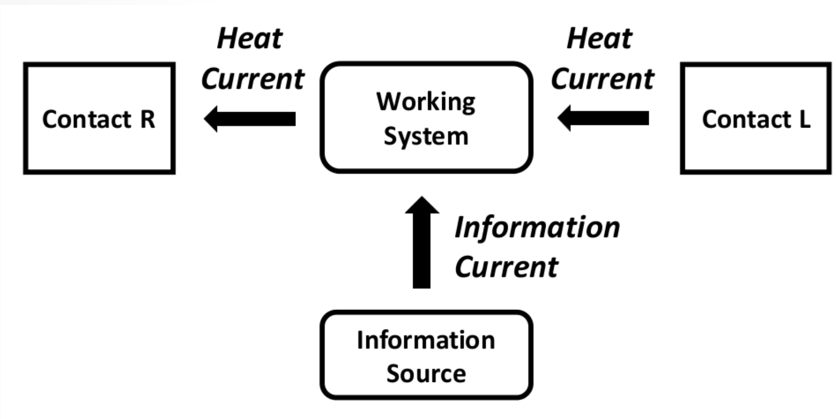


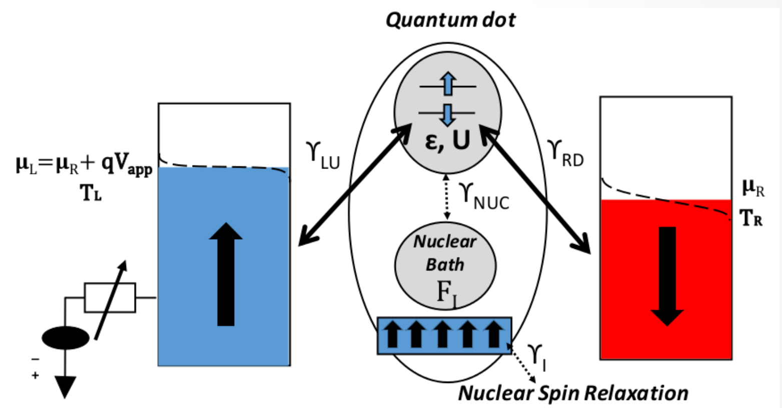




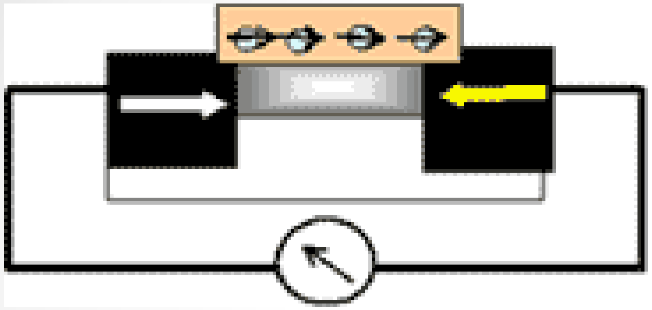


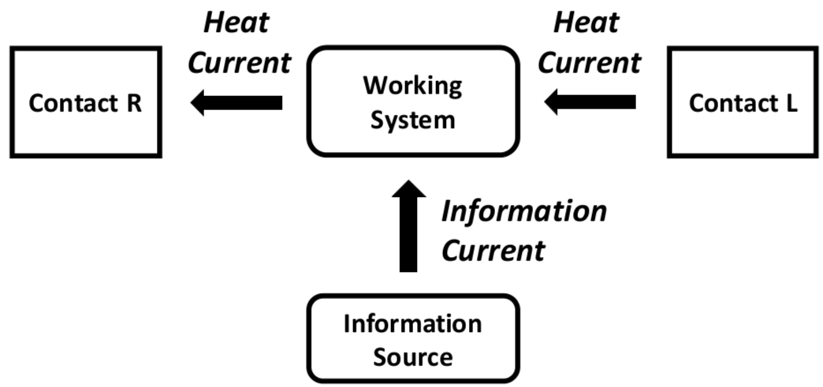
Part III: Information driven thermal machine





Landauer writing and erasure

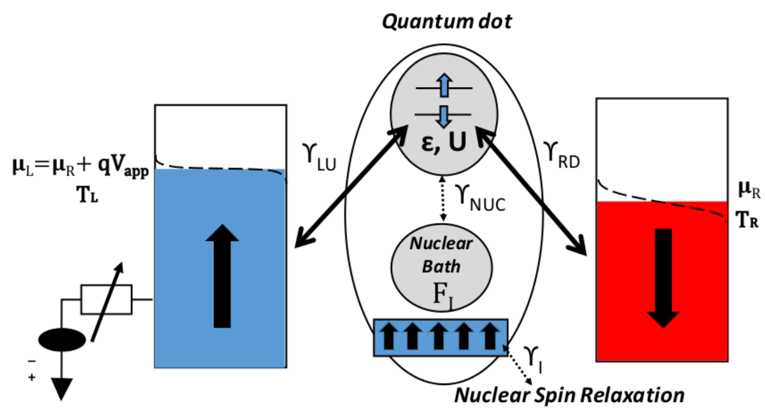




$$N_1 + N_2 = 0$$

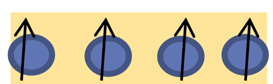
$$E_1 + E_2 + E_0 = 0$$

$$\frac{E_1 - \mu_1 N_1}{T_1} + \frac{E_2 - \mu_2 N_2}{T_2} - \Delta S_0 \leq 0$$

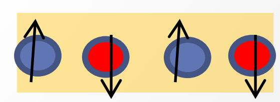


$$\Delta S_{tot} \geq 0$$

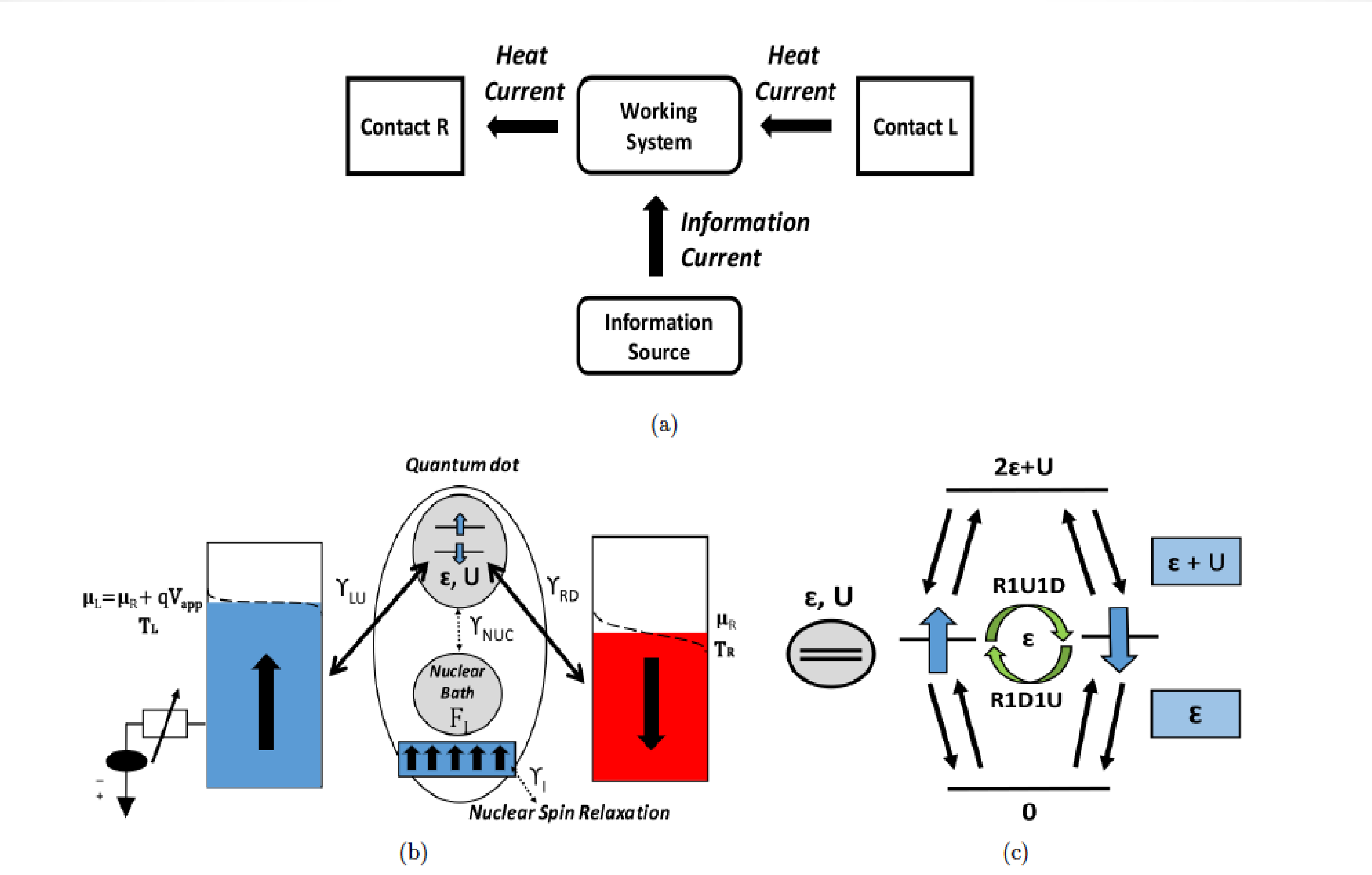
$$\Delta F = \underbrace{\Delta E}_{\text{ENERGY}} - \underbrace{T\Delta S}_{\text{INFORMATION}} \leq 0$$



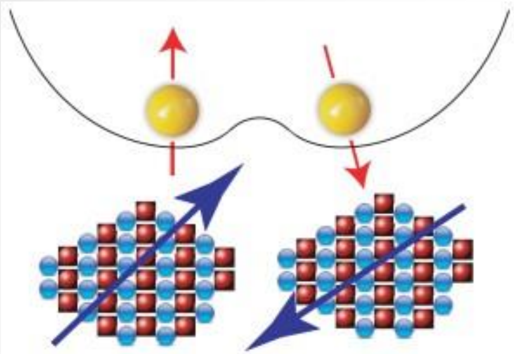
v/s



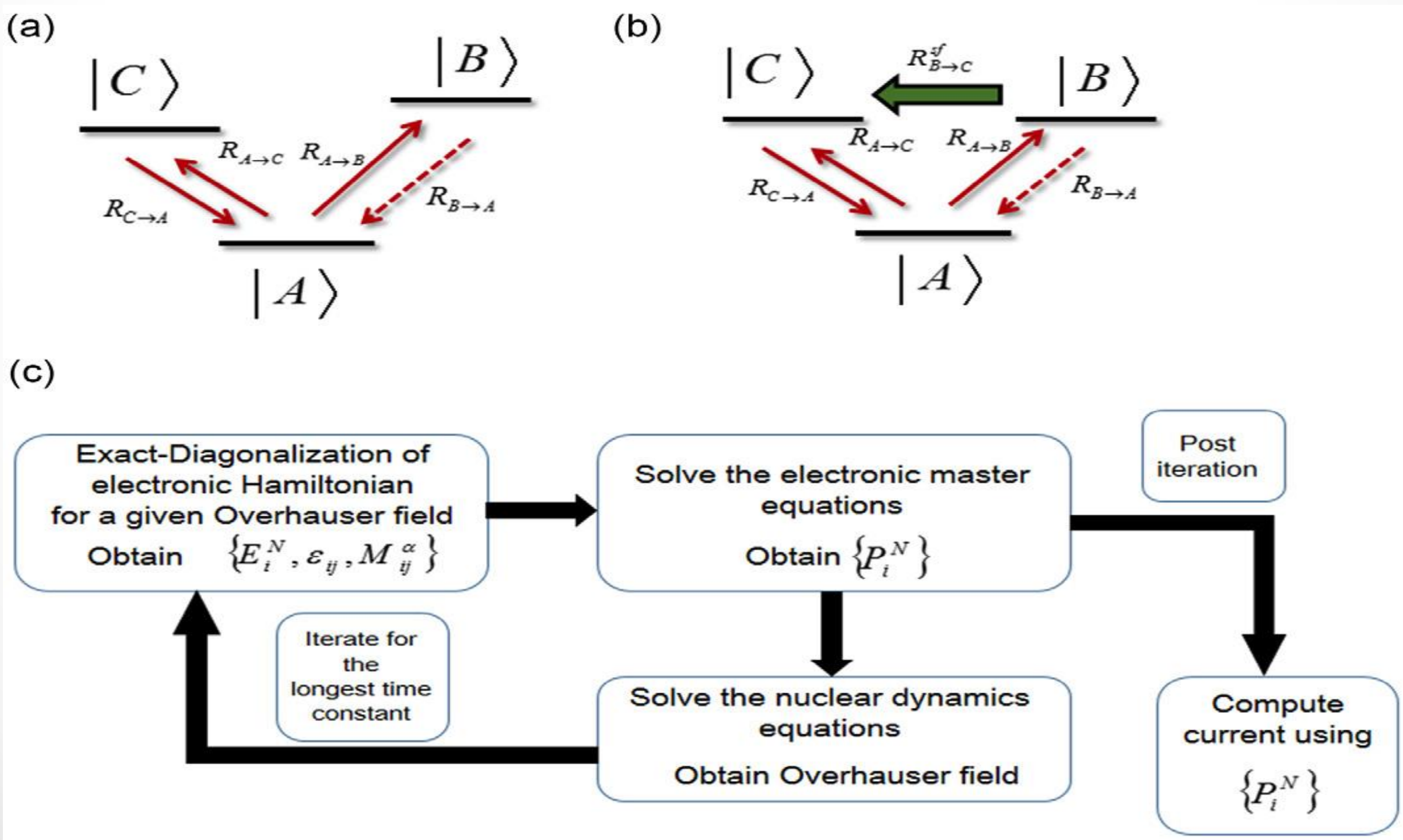
Hyperfine thermal machine



Hyperfine interaction basics



$$\hat{H}_{HF}(\mathbf{r}_n) = \sum_n A_{eff}\,\psi^*(\mathbf{r}_n)\psi(\mathbf{r_n})\mathbf{a}_0^3\left[\hat{\mathbf{S}}_\mathbf{z} \otimes \hat{\mathbf{I}}^\mathbf{n}_\mathbf{z} + \left\{\frac{\hat{\mathbf{I}}^\mathbf{n}_+ \otimes \hat{\mathbf{S}}_- + \hat{\mathbf{S}}_+ \otimes \hat{\mathbf{I}}^\mathbf{n}_-}{\mathbf{2}}\right\}\right]$$

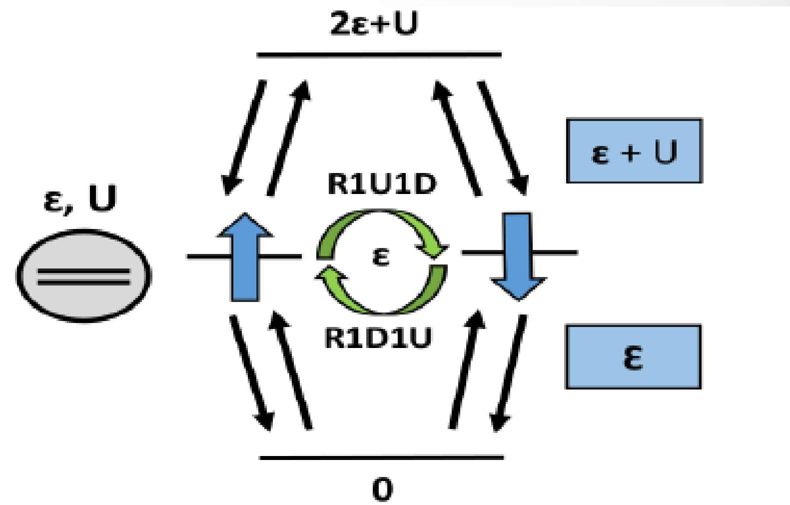


SQD: Basic Formulation

$$\frac{dP_0^0}{dt} = -R_{(0,0)\to(1,\uparrow)}P_0^0 - R_{(0,0)\to(1,\downarrow)}P_0^0 + R_{(1,\uparrow)\to(0,0)}P_\uparrow^1 + R_{(1,\downarrow)\to(0,0)}P_\downarrow^1$$

$$\frac{dP_\uparrow^1}{dt} = -R_{(1,\uparrow)\to(0,0)}P_\uparrow^1 - R_{(1,\uparrow)\to(2,0)}P_\uparrow^1 + R_{(2,0)\to(1,\uparrow)}P_0^2 + R_{(0,0)\to(1,\uparrow)}P_0^0 + R^{sf}_{(1,\downarrow)\to(1,\uparrow)}P_\downarrow^1 - R^{sf}_{(1,\uparrow)\to(1,\downarrow)}P_\uparrow^1$$

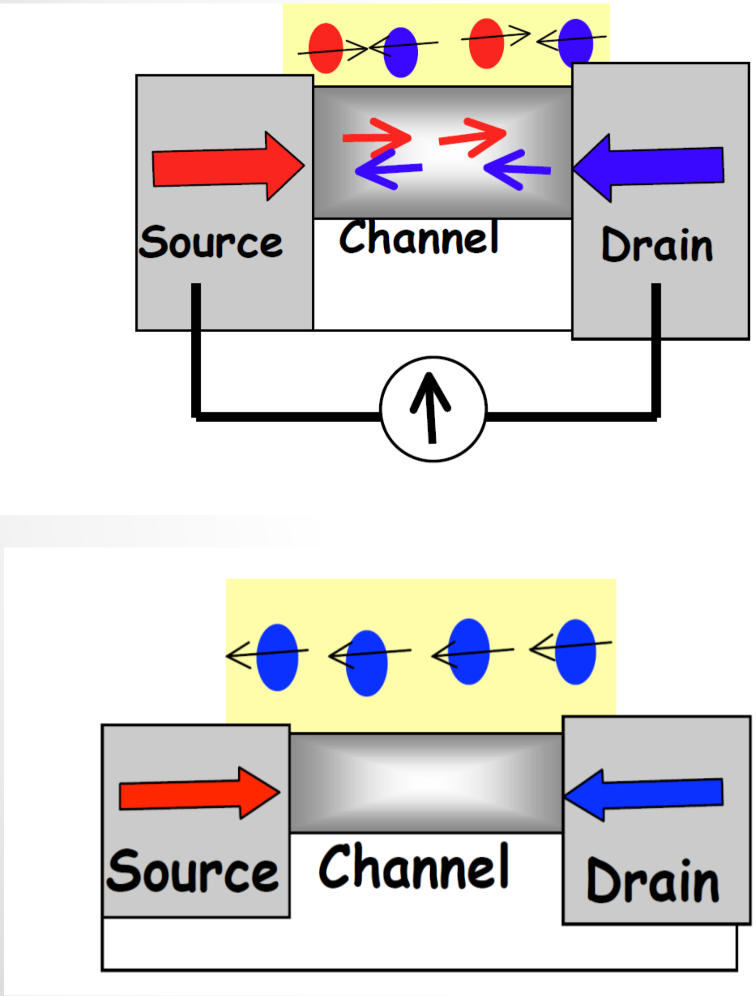
$$\frac{dP_\downarrow^1}{dt} = -R_{(1,\downarrow)\to(0,0)}P_\downarrow^1 - R_{(1,\downarrow)\to(2,0)}P_\downarrow^1 + R_{(2,0)\to(1,\downarrow)}P_0^2 + R_{(0,0)\to(1,\downarrow)}P_0^0 + R^{sf}_{(1,\uparrow)\to(1,\downarrow)}P_\uparrow^1 - R^{sf}_{(1,\downarrow)\to(1,\uparrow)}P_\downarrow^1$$

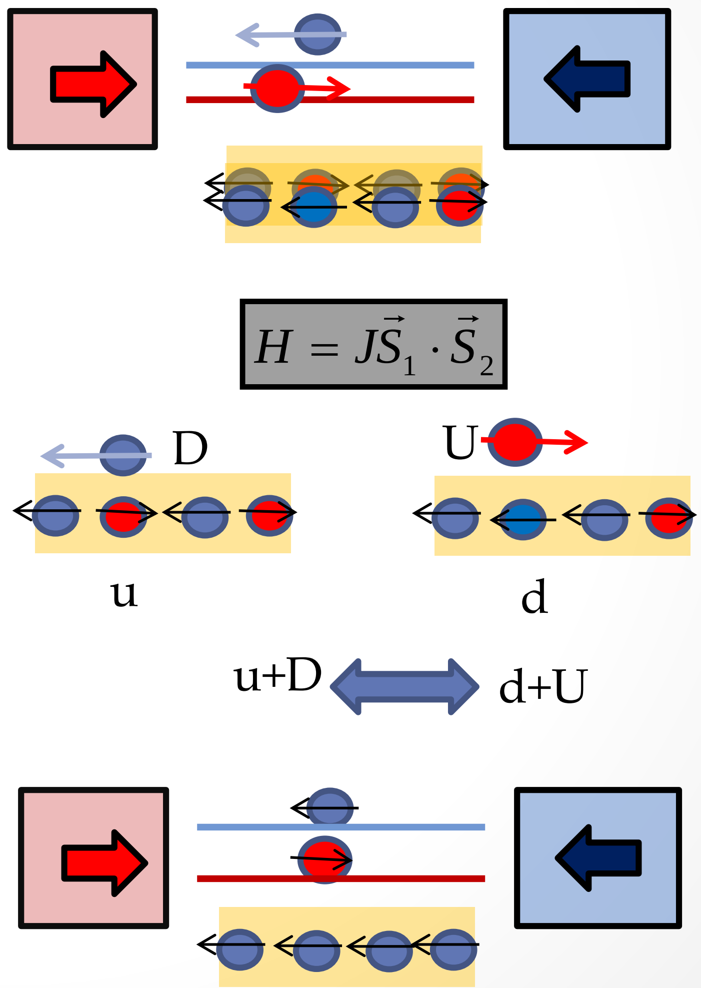


$$\frac{dF_I}{dt} = \gamma^{nuc}[(P_\uparrow^1 - P_\downarrow^1) - (P_\uparrow^1 + P_\downarrow^1)F_I] - \gamma_I F_I$$

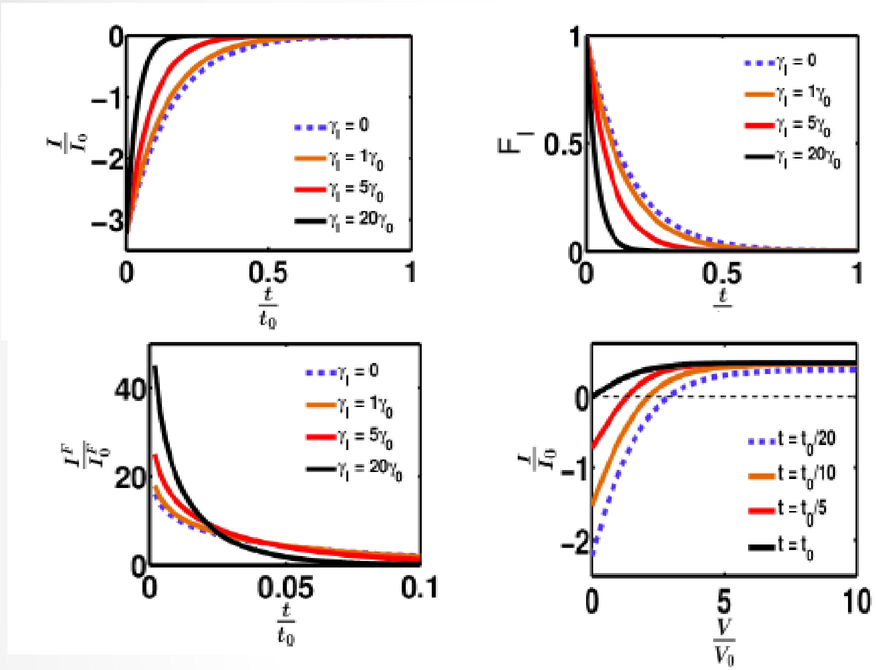
$$\frac{dS_I}{dt} = k_b \frac{1}{2} ln \frac{1+F_I}{1-F_I}\left(\gamma^{nuc}[(P_\uparrow^1 - P_\downarrow^1) - (P_\uparrow^1 + P_\downarrow^1)F_I] - \gamma_I F_I\right)$$

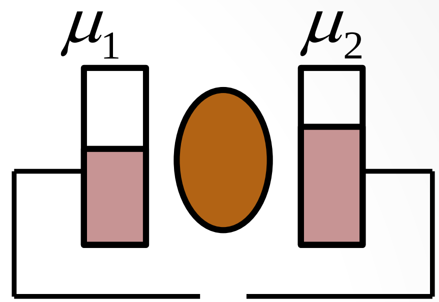
nano-device “demons”+ info battery





nano-device "demons"+ info battery





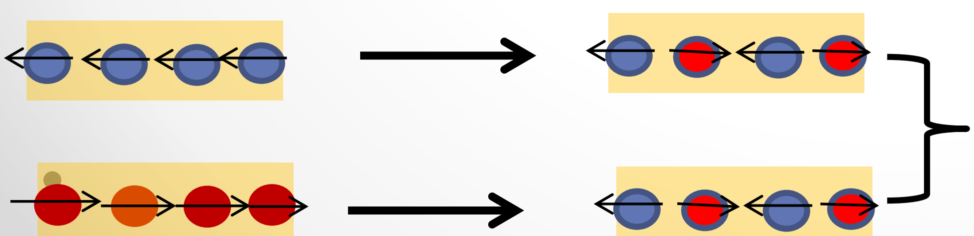
$$\boxed{\begin{aligned} S_i &= 0 \\ S_f &= Nk \ln 2 \\ \Delta S &= Nk \ln 2 \\ \Delta W &\le NkT \ln 2 \end{aligned}}$$

$$\boxed{\begin{aligned} S_i &= 0 \\ S_f &= Nk \ln 2 \\ \Delta S &= Nk \ln 2 \end{aligned}}$$

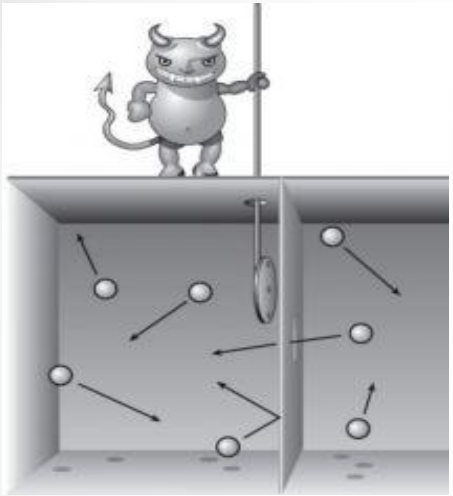
Current Stops to flow eventually!

Where does the energy come from?!

State of the Demons



Connection with Maxwell's Demon



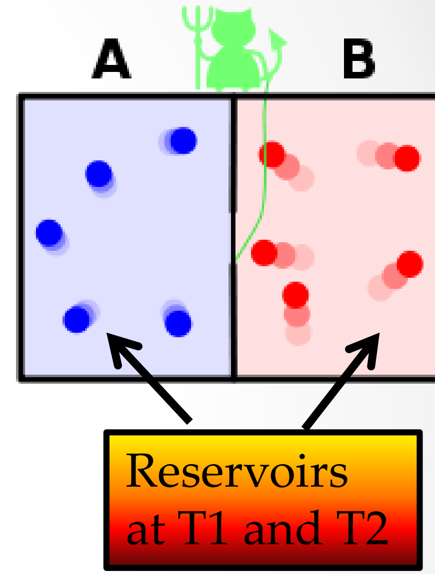
ON THE DECREASE OF ENTROPY IN A THERMODYNAMIC SYSTEM BY THE INTERVENTION OF INTELLIGENT BEINGS

LEO SZILARD

Translated by Anatol Rapoport and Mechthilde Knoller from the original article "Über die Entropieverminderung in einem thermodynamischen System bei Eingriffen intelligenter Wesen." Zeitschrift für Physik, 1929, 53, 840–856

The objective of the investigation is to find the conditions which apparently allow the construction of a perpetual-motion machine of the second kind, if one permits an intelligent being to intervene in a thermodynamic system. When such beings make measurements, they make the system behave in a manner distinctly different from the way a mechanical system behaves when left to itself. We show that it is a sort of a memory faculty, manifested by a system where measurements occur, that might cause a permanent decrease of entropy and thus a violation of the Second Law of Thermodynamics, were it not for the fact that the measurements themselves are necessarily accompanied by a production of entropy. At first we calculate this production of entropy quite generally from the postulate that full compensation is made in the sense of the Second Law (Equation [1]). Second, by using an inanimate device able to make measurements—however under continual entropy production—we shall calculate the resulting quantity of entropy. We find that it is exactly as great as is necessary for full compensation. The actual production of entropy in connection with the measurement, therefore, need not be greater than Equation (1) requires.

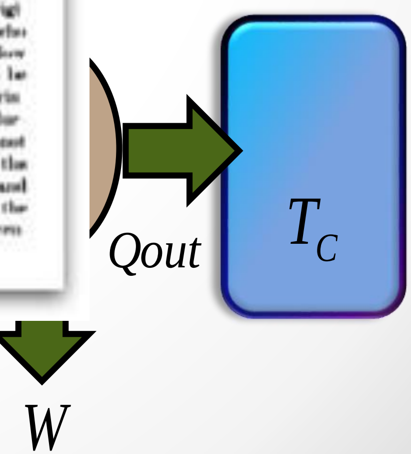
There is an objection, already historical, against the universal validity of the Second Law of Thermodynamics, which indeed looks rather ominous. The objection is embodied in the notion of Maxwell's demon, who in a different form appears even nowadays again and again; perhaps not unreasonably, inasmuch as behind the precisely formulated question quantitative connections seem to be hidden which to date have not been clarified. The objection in its original formulation concerns a demon who catches the fast molecules and lets the slow ones pass. To be sure, the objection can be met with the reply that man cannot in principle foresee the value of a thermally fluctuating parameter. However, one cannot deny that we can very well measure the value of such a fluctuating parameter and therefore could certainly gain energy at the expense of heat by arranging our interven



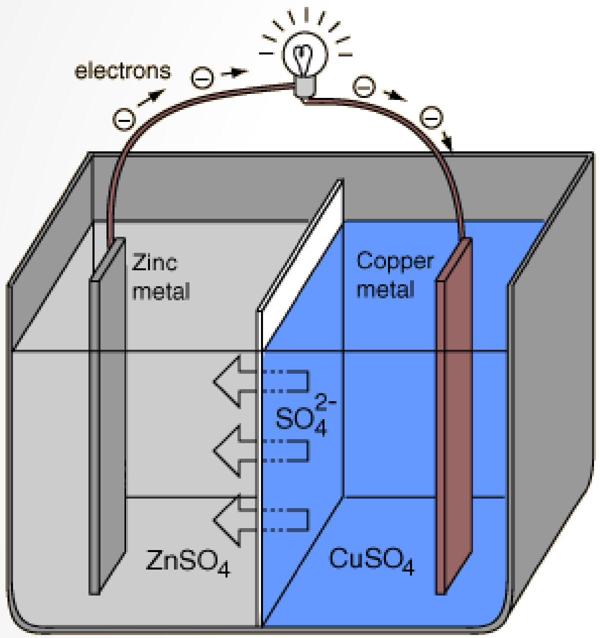
Does it no violate an
Common sense?

If not, what is the ca

Demon exorcism by

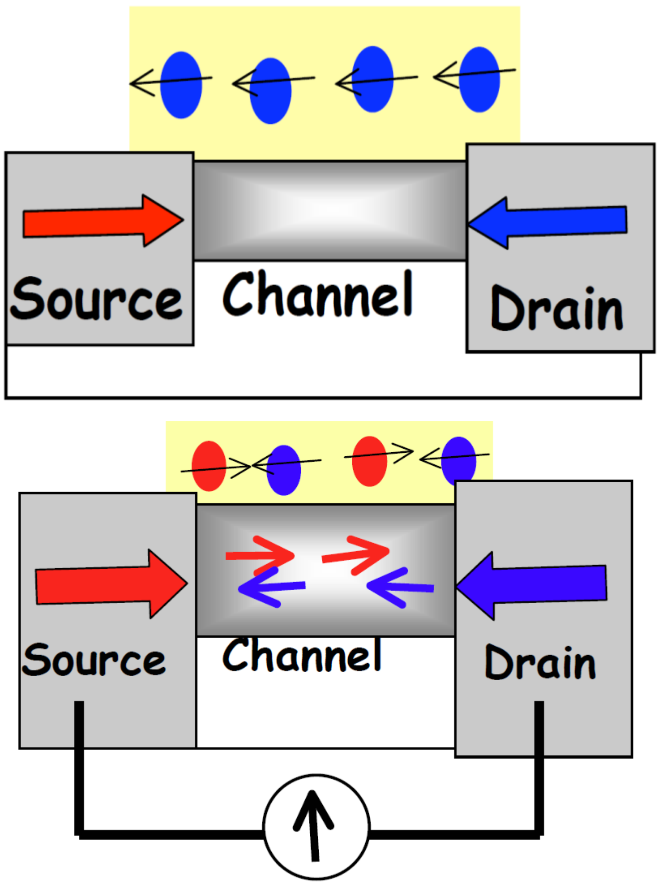


Connection with Maxwell's demon



$$\Delta S_{tot} \geq 0$$

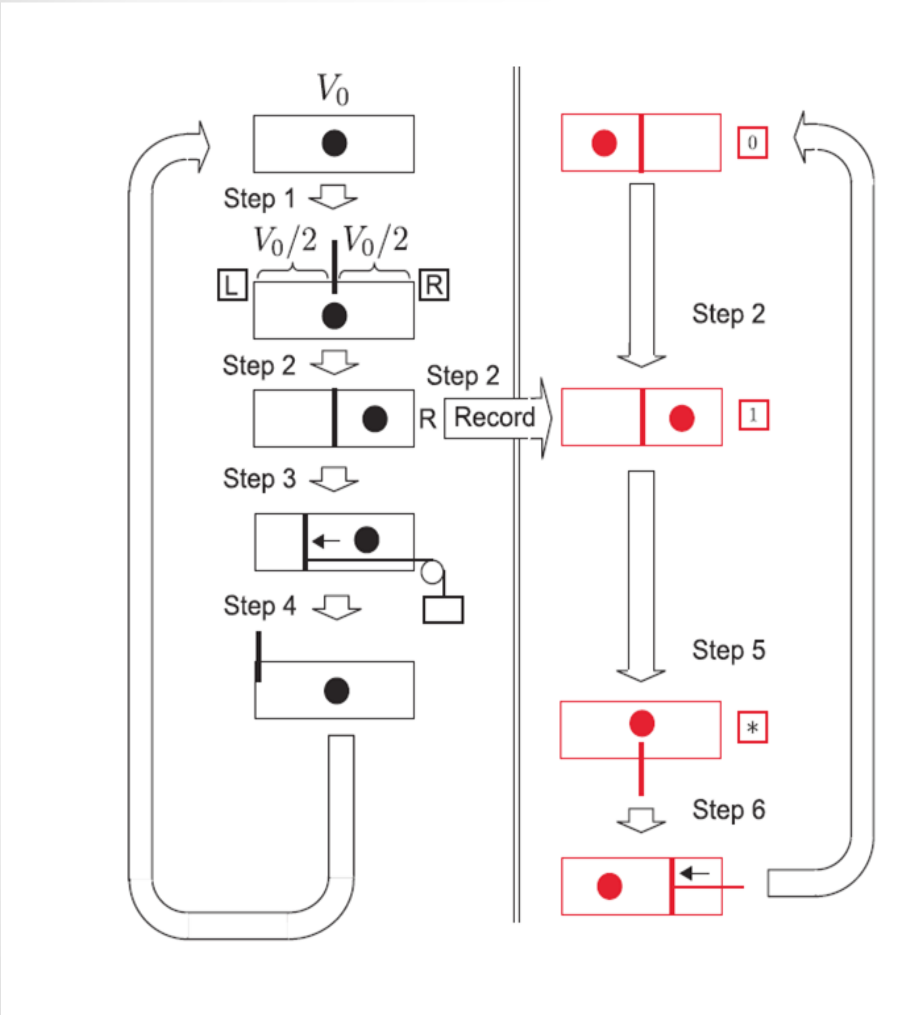
$$\underbrace{\Delta F = \Delta E}_{\text{Energy}} - T\Delta S \leq 0$$



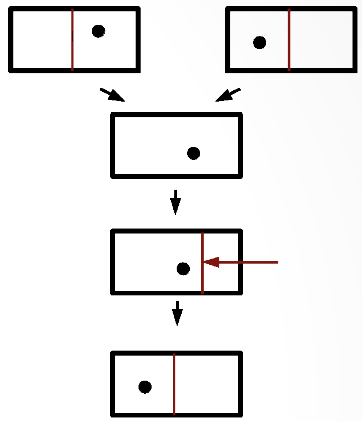
$$\Delta S_{tot} \geq 0$$

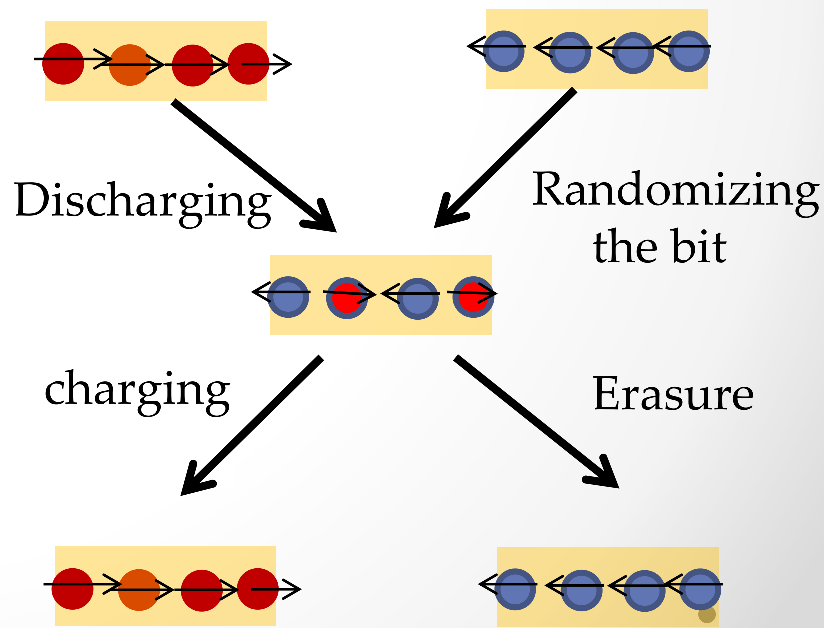
$$\Delta F = \Delta E - \underbrace{T\Delta S}_{\text{Information}} \leq 0$$

Connection with Maxwell's demon/Landauer principle



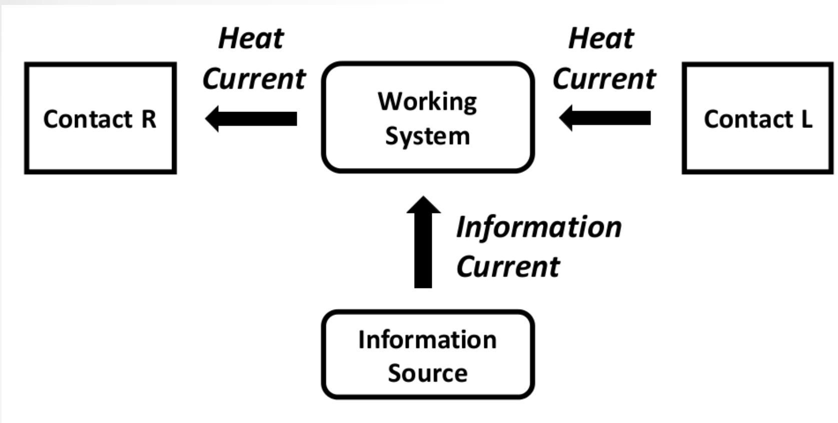
State of the Demons

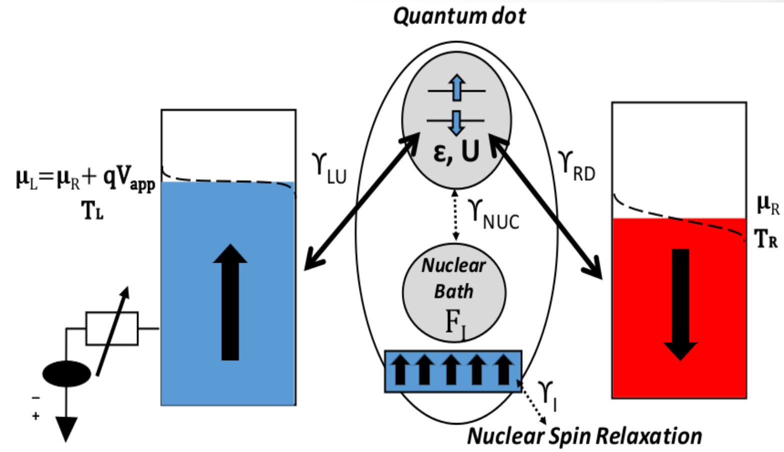


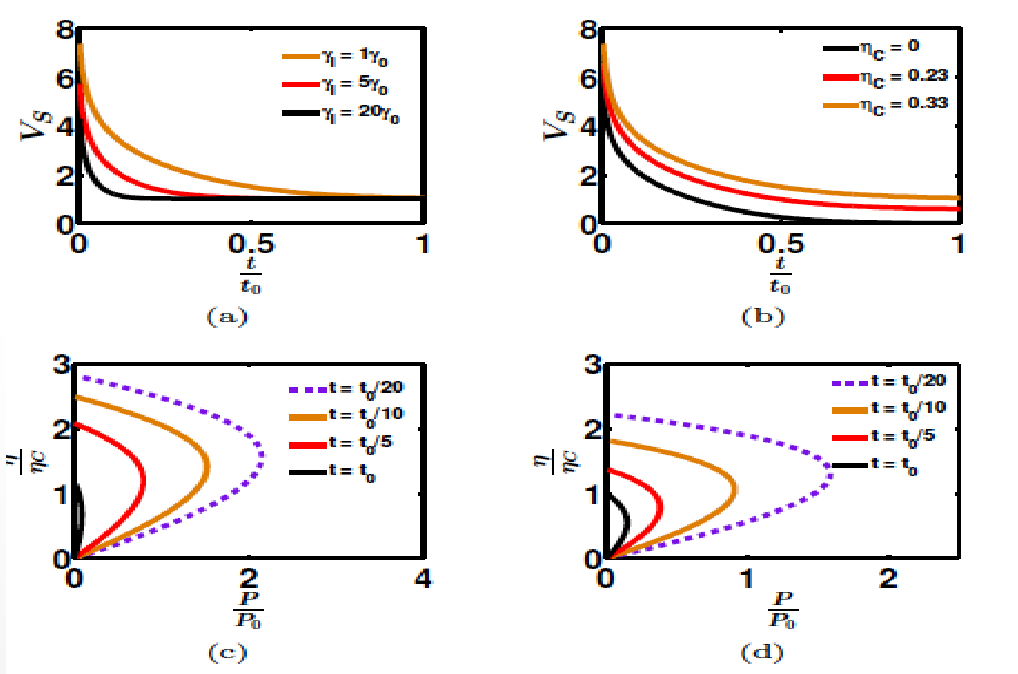


$$\Delta S = Nk \ln 2$$
$$\Delta W \leq NkT \ln 2$$
$$E_{Erase} \geq NkT \ln 2$$

Information flow: Larger than Carnot operation

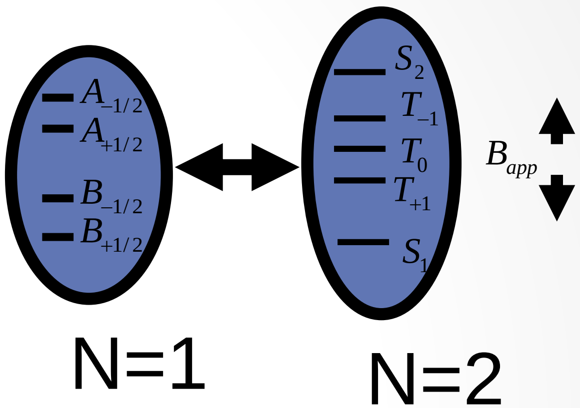


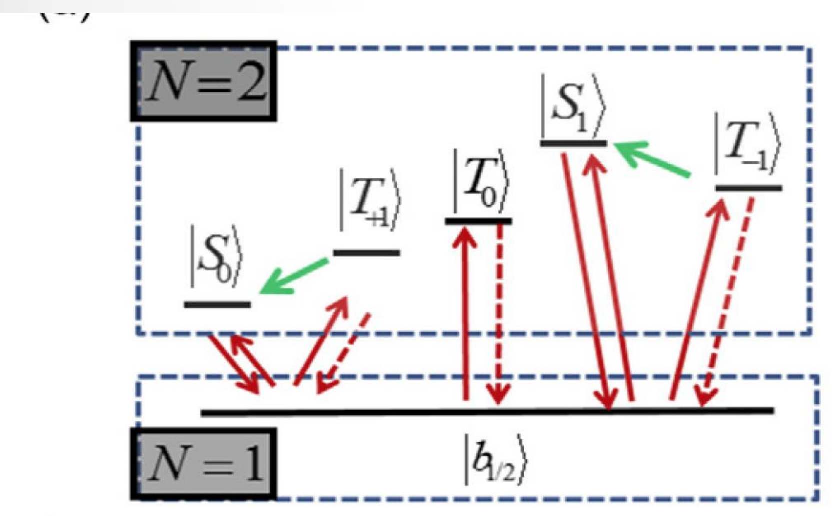


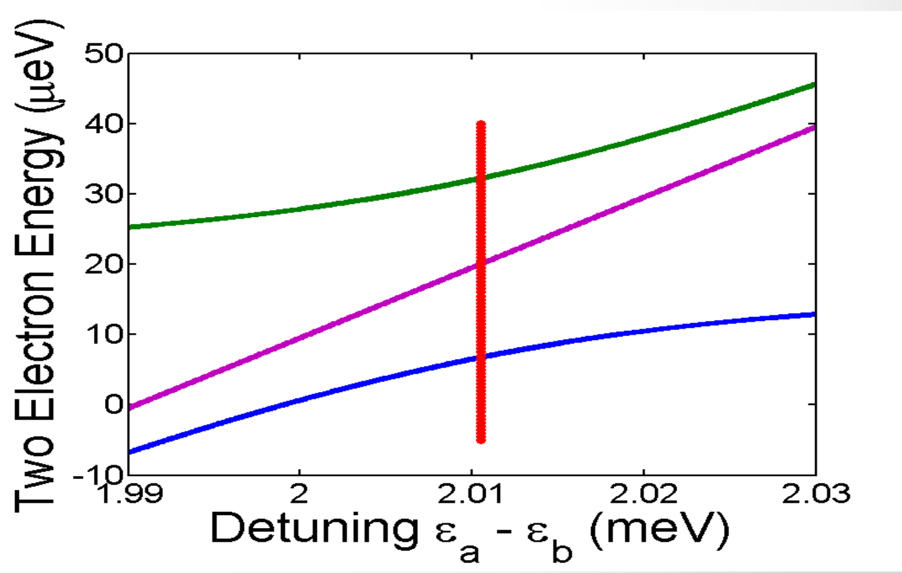


PSB Application: Double Resonance due to Two-Electron states

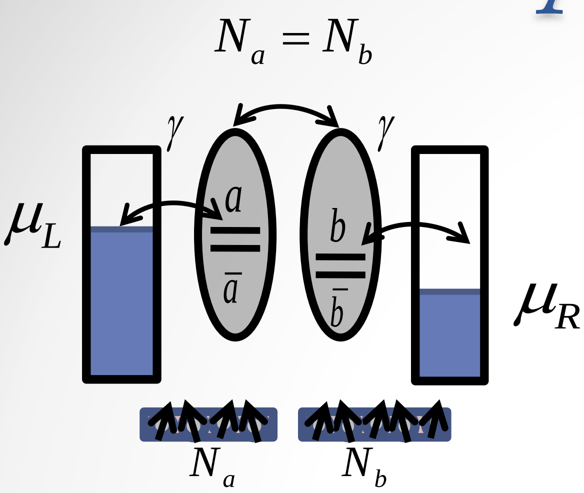
- Two-electron states at **B = 0**
  - Three S = 1 states *(T)*
  - Three S = 0 states *(S)*
- Triplets are blocking states
- **TWO RESONANCES**:
  - $\boldsymbol{T_{+1} - S_1}$
  - $\boldsymbol{T_{-1} - S_2}$
- T_+ *and* T_- move in opposite directions under **B** and $\mathbf{F_I}$.





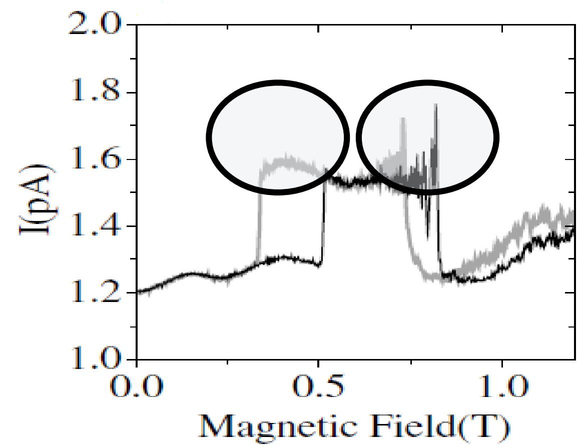


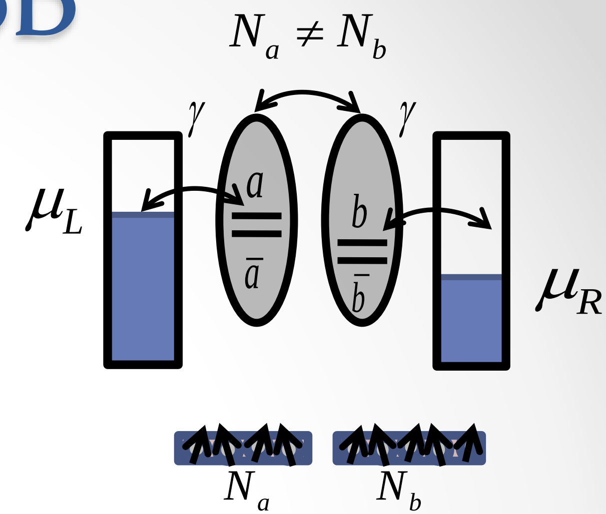
Applied to PSB



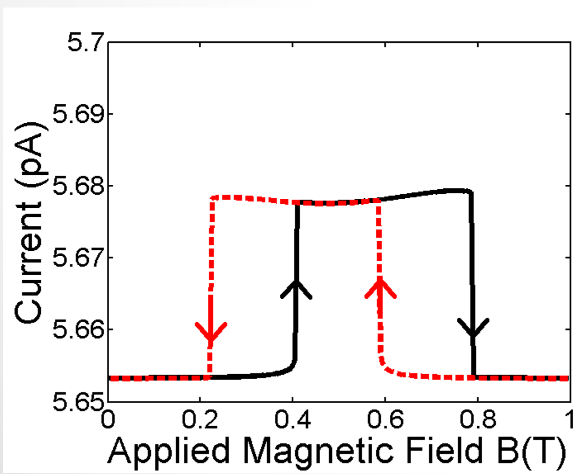
K. Ono et al. PRL 04

EXPERIMENT



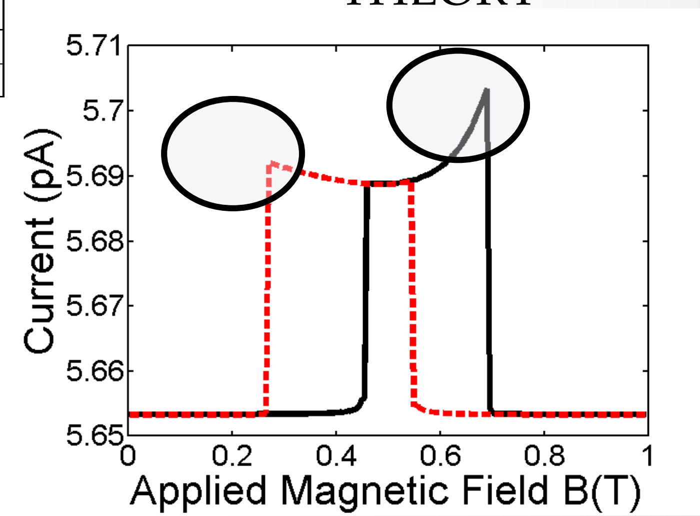


THEORY



Fin Structure

THEORY



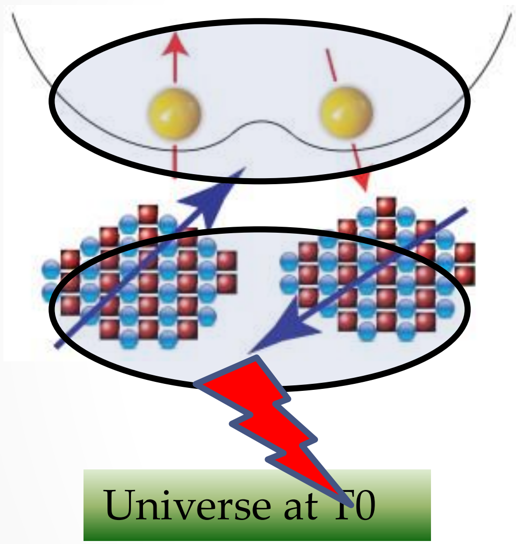
Dual Resonance

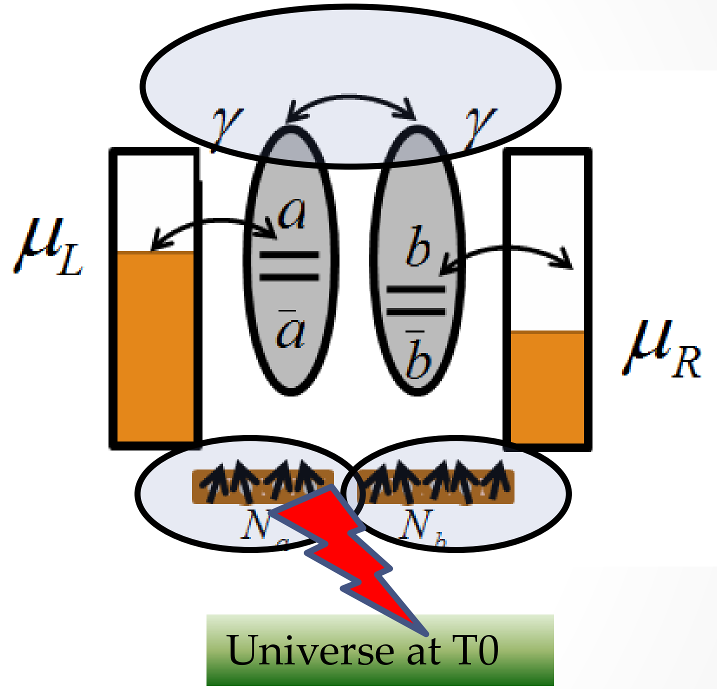
Un-identical baths

S Buddhiraju and B Muralidharan, JPCM, 26, 485302, (2014)

Other "complicated" nanoscale demons
The case of Entanglement and quantum information:

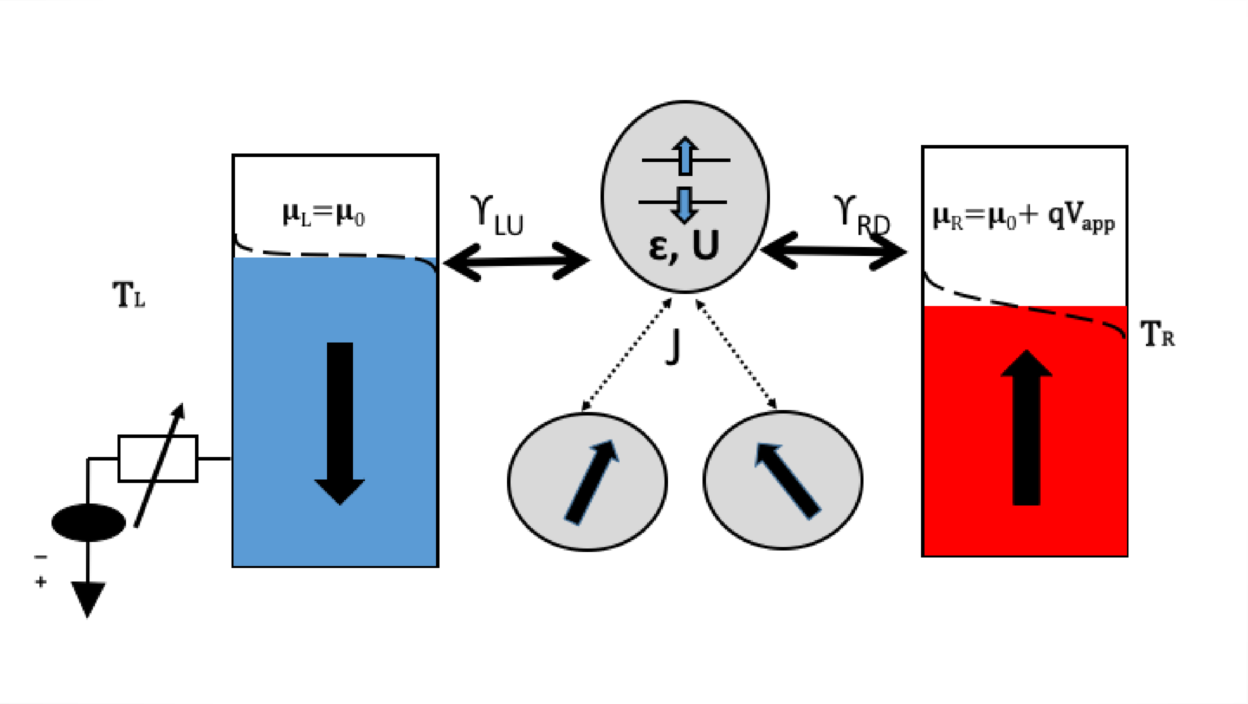
$$S = Tr[\rho \ln \rho]$$



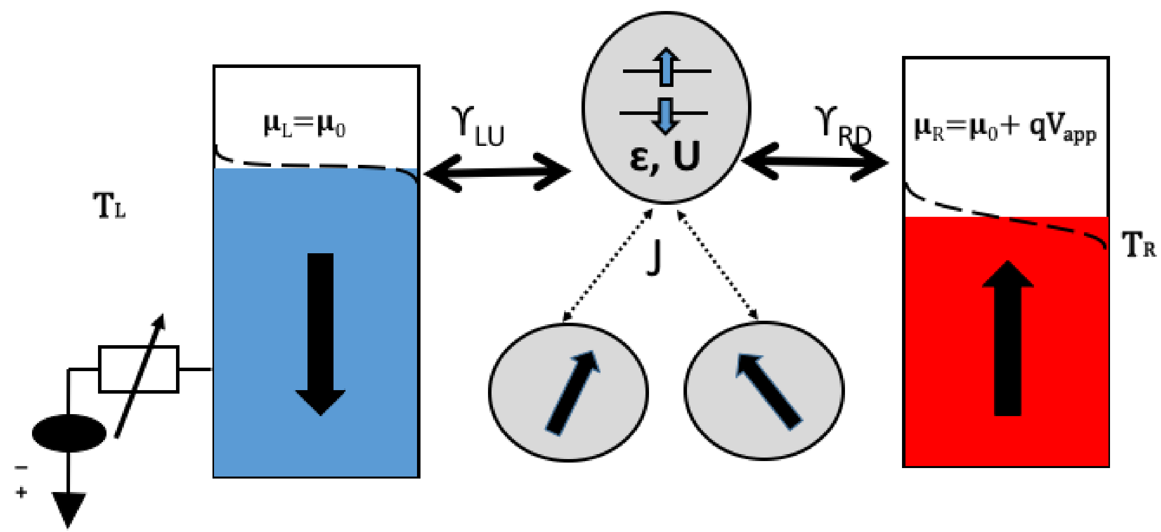


$$|2,i\rangle = \alpha_{0/1}|a\bar{b}\rangle + \beta_{0/1}|\bar{a}b\rangle + \xi_{0/1}|a\bar{a}\rangle + \delta_{0/1}|b\bar{b}\rangle$$

Part IV: Concurrence Thermal Machines



Set up and Many-body states



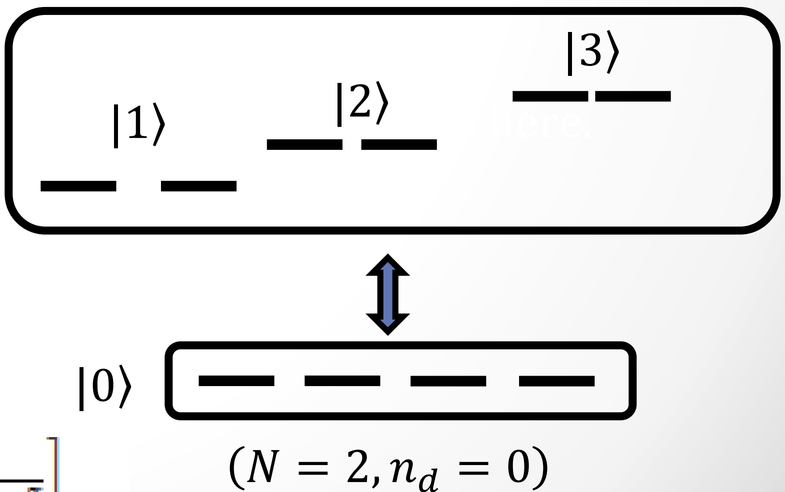
)

$$H_S = \sum_{\sigma=\uparrow,\downarrow} \hbar\omega_\sigma \hat{n}_\sigma + U\hat{n}_\uparrow \hat{n}_\downarrow + \hbar J \mathbf{S}_{dot} \cdot (\mathbf{S}_1 + \mathbf{S}_2)$$

$$H_T = \hbar \sum_{\alpha k \sigma} \left(t_{\alpha k \sigma} c^\dagger_{\alpha k \sigma} d_\sigma + \text{H.C.} \right)$$

$$H_C = \sum_{\alpha k \sigma} (\epsilon_{\alpha k \sigma} \hat{n}_{\alpha k \sigma}) = \hbar \sum_{\alpha k \sigma} \left(\omega_{\alpha k \sigma} c^\dagger_{\alpha k \sigma} c_{\alpha k \sigma} \right)$$

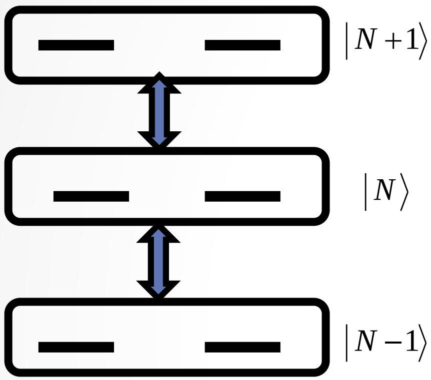
$$H_1 = \frac{\hbar}{4\pi} P \int d\xi \sum_\alpha (1 - 2f_\alpha(\xi)) \times \left[\frac{\gamma_\alpha \gamma_\alpha^\dagger}{\varepsilon_1 - \varepsilon_0 - \xi} - \frac{\gamma_\alpha \gamma_\alpha^\dagger}{\varepsilon_2 - \varepsilon_1 - \xi} \right]$$



Density Matrix master equations

For constant density of states we define:

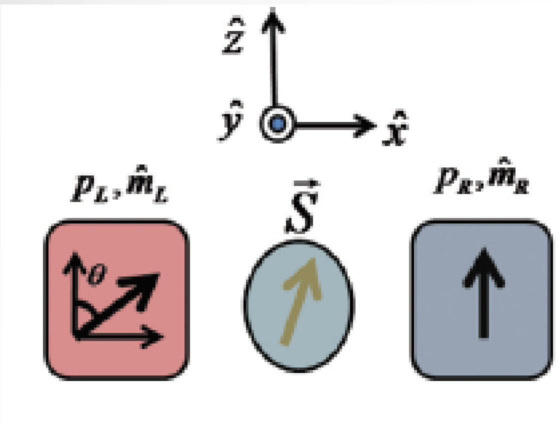
$$\Gamma_{\alpha\sigma_\alpha} = \frac{2\pi D_{\alpha k\sigma_\alpha}\left|t_\alpha\right|^2}{\hbar}$$

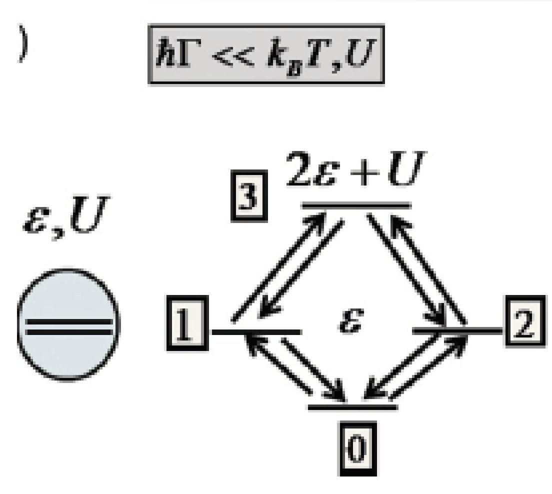


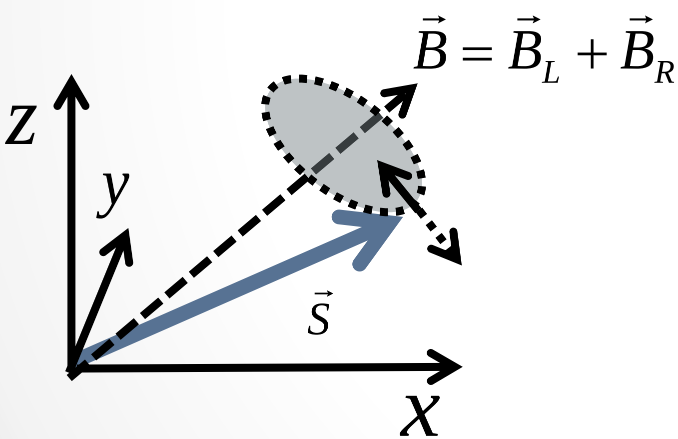
The equations then become:

$$\dot{\rho}_{nm}^{E_N N}(t) = -\sum_{\alpha\sigma_\alpha}\left\{\sum_{l,l'\in|N-1\rangle}\ \sum_{j\in|E_N,N\rangle}\ \sum_{h,h'\in|N+1\rangle}\right\}\frac{\Gamma_{\alpha\sigma_\alpha}}{2}\left\{\begin{array}{l}
\left[\overbrace{f_\alpha(\varepsilon_h-\varepsilon_j)}^{\text{Real transitions}}+\frac{i}{\pi}\int d\varepsilon_k\,\overbrace{\frac{f_\alpha(\varepsilon_k)}{\varepsilon_k-\varepsilon_h+\varepsilon_j}}^{\begin{matrix}\text{Virtual transitions}\\ \text{Energy non-conserving}\end{matrix}}\right]M_{nh}^{\alpha\sigma_\alpha}(M_{hj}^{\alpha\sigma_\alpha})^*\rho_{jm}^{E_N N}\\
+\left[\left(1-f_\alpha(\varepsilon_j-\varepsilon_l)\right)-\frac{i}{\pi}\int d\varepsilon_k\frac{(1-f_\alpha(\varepsilon_k))}{\varepsilon_k-\varepsilon_j+\varepsilon_l}\right](M_{nl}^{\alpha\sigma_\alpha})^* M_{lj}^{\alpha\sigma_\alpha}\rho_{jm}^{E_N N}\\
+\left[f_\alpha(\varepsilon_h-\varepsilon_j)-\frac{i}{\pi}\int d\varepsilon_k\frac{f_\alpha(\varepsilon_k)}{\varepsilon_k-\varepsilon_h+\varepsilon_j}\right]\rho_{nj}^{E_N N}M_{jh}^{\alpha\sigma_\alpha}(M_{hm}^{\alpha\sigma_\alpha})^*\\
+\left[\left(1-f_\alpha(\varepsilon_j-\varepsilon_l)\right)+\frac{i}{\pi}\int d\varepsilon_k\frac{(1-f_\alpha(\varepsilon_k))}{\varepsilon_k-\varepsilon_j+\varepsilon_l}\right]\rho_{nj}^{E_N N}(M_{jl}^{\alpha\sigma_\alpha})^* M_{lm}^{\alpha\sigma_\alpha}\\
-2(1-f_\alpha(\varepsilon_h-\varepsilon_j))M_{nh'}^{\alpha\sigma_\alpha}\rho_{h'h}^{E_h N+1}(M_{hm}^{\alpha\sigma_\alpha})^*\\
-f_\alpha(\varepsilon_j-\varepsilon_l)M_{nl'}^{\alpha\sigma_\alpha}\rho_{l'l}^{E_l N-1}(M_{lm}^{\alpha\sigma_\alpha})^*
\end{array}\right\}$$

Example of Density Matrix-Coherences







$$\vec{J}^{\,S}_{\alpha} = \left[\underbrace{\frac{\hbar}{2q} J^{q}_{\alpha} p_{\alpha} \hat{m}_{\alpha}}_{\text{Injection}} - \underbrace{\frac{\vec{S} - p_{\alpha}^{2}\left(\hat{m}_{\alpha} \cdot \vec{S}\right)\hat{m}_{\alpha}}{\tau_{r,\alpha}}}_{\text{Relaxation}} + \underbrace{\vec{S} \times \vec{B}_{\alpha}}_{\text{Precession}} \right]$$

Koenig and Martinek PRL (2004).

B. Muralidharan and M Grifoni,
Phys. Rev. B, 88, 045402, (2013).

Density Matrix master equations

$$\nu^{+}_{\alpha;k,k'} = \langle k,\cdot|t^{*}_{\alpha}d^{\dagger}_{\alpha}|k',\cdot\rangle$$

$$(\nu^{+}_{\alpha;k,k'})^{\dagger} = \nu^{-}_{\alpha;k',k}$$

$$\nu^{-}_{\alpha;k,k'} = \langle k,\cdot|t_{\alpha}d_{\alpha}|k',\cdot\rangle$$

$$\gamma^{\pm}_{\alpha;k,k'} = \left(\frac{2\pi D_{\alpha}}{\hbar}\right)^{1/2}\nu^{\pm}_{\alpha;k,k'}$$

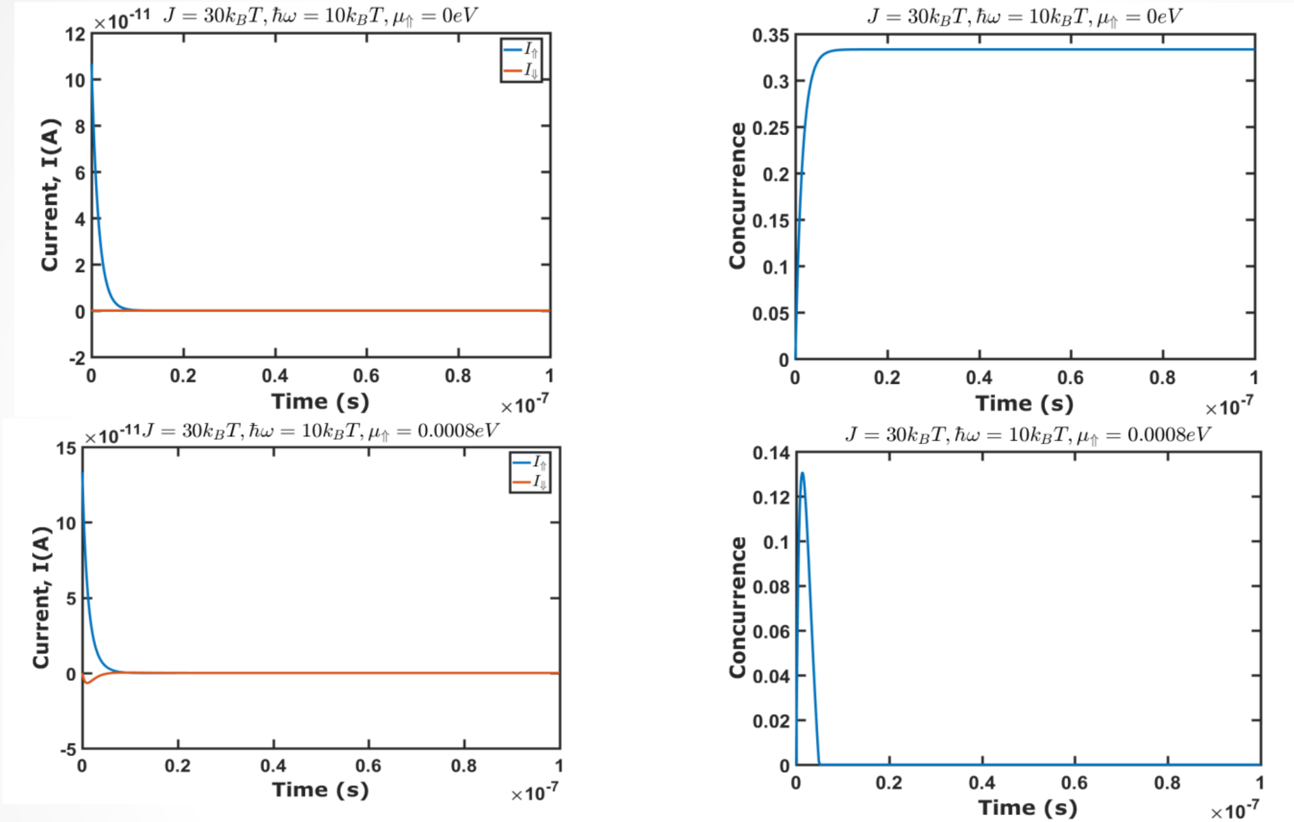
$$H_1 = \frac{\hbar}{4\pi}P\int d\xi\sum_{\alpha}(1-2f_{\alpha}(\xi))\times\left[\frac{\gamma_{\alpha}\gamma^{\dagger}_{\alpha}}{\varepsilon_1-\varepsilon_0-\xi}-\frac{\gamma_{\alpha}\gamma^{\dagger}_{\alpha}}{\varepsilon_2-\varepsilon_1-\xi}\right]$$

$$\dot{\rho}_0 = \frac{i}{\hbar}[\rho_0,H_0]+\sum_{\alpha}\sum_{k\in\{a,b,c\}}(1-f_{\alpha}(E_k-E_0))\,\gamma^{-}_{\alpha;0,k}\rho_k\gamma^{+}_{\alpha;k,0}-\frac{1}{2}f_{\alpha}(E_k-E_0)\left\{\rho_0,\gamma^{-}_{\alpha;0,k}\gamma^{+}_{\alpha;k,0}\right\}$$

$$\dot{\rho}_2 = \frac{i}{\hbar}[\rho_2,H_2]+\sum_{\alpha}\sum_{k\in\{a,b,c\}}f_{\alpha}(E_2-E_k)\gamma^{+}_{\alpha;2,k}\rho_k\gamma^{-}_{\alpha;k,2}-\frac{1}{2}(1-f_{\alpha}(E_2-E_k))\left\{\rho_2,\gamma^{+}_{\alpha;2,k}\gamma^{-}_{\alpha;k,2}\right\}$$

$$\begin{aligned}\dot{\rho}_k = {}&\frac{i}{\hbar}[\rho_k,H_k]+\sum_{\alpha}f_{\alpha}(E_k-E_0)\gamma^{+}_{\alpha;k,0}\rho_0\gamma^{-}_{\alpha;0,k}-\frac{1}{2}(1-f_{\alpha}(E_k-E_0))\left\{\rho_k,\gamma^{+}_{\alpha;k,0}\gamma^{-}_{\alpha;0,k}\right\}\\&+\sum_{\alpha}(1-f_{\alpha}(E_2-E_k))\,\gamma^{-}_{\alpha;k,2}\rho_2\gamma^{+}_{\alpha;2,k}-\frac{1}{2}f_{\alpha}(E_2-E_k)\left\{\rho_k,\gamma^{-}_{\alpha;k,2}\gamma^{+}_{\alpha;2,k}\right\}\end{aligned}$$

Battery/Power Source Functionality

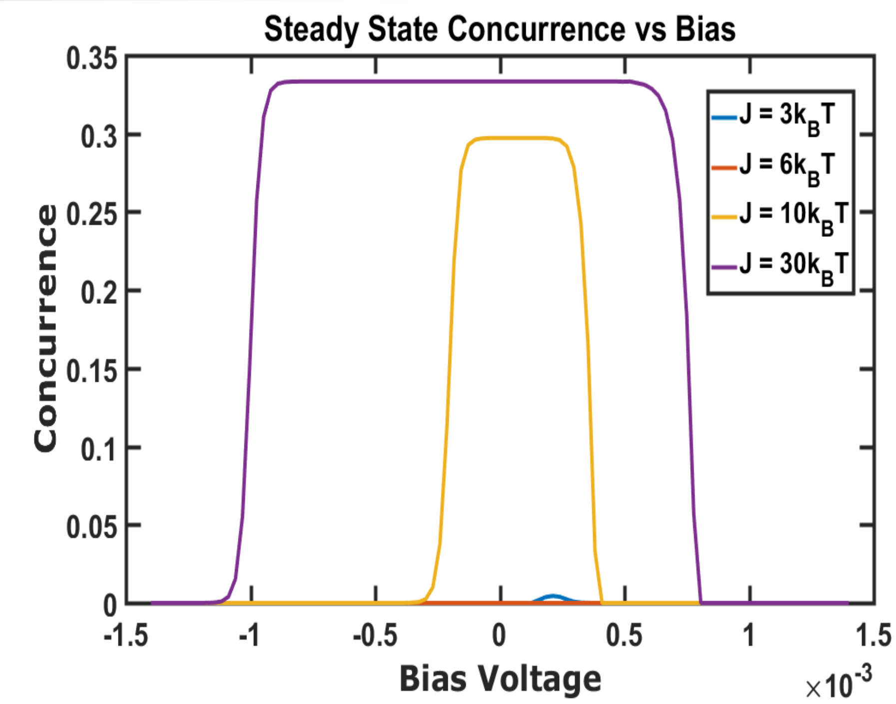


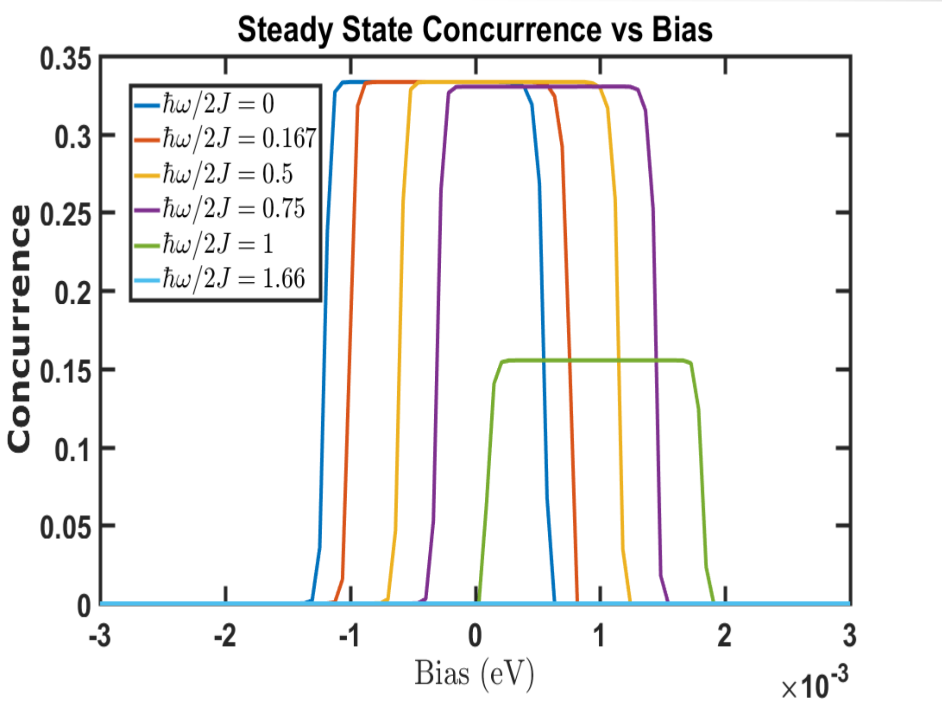
$$C(\rho) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4),$$

where λ_i are the eigenvalues, in decreasing order, of the Hermitian operator

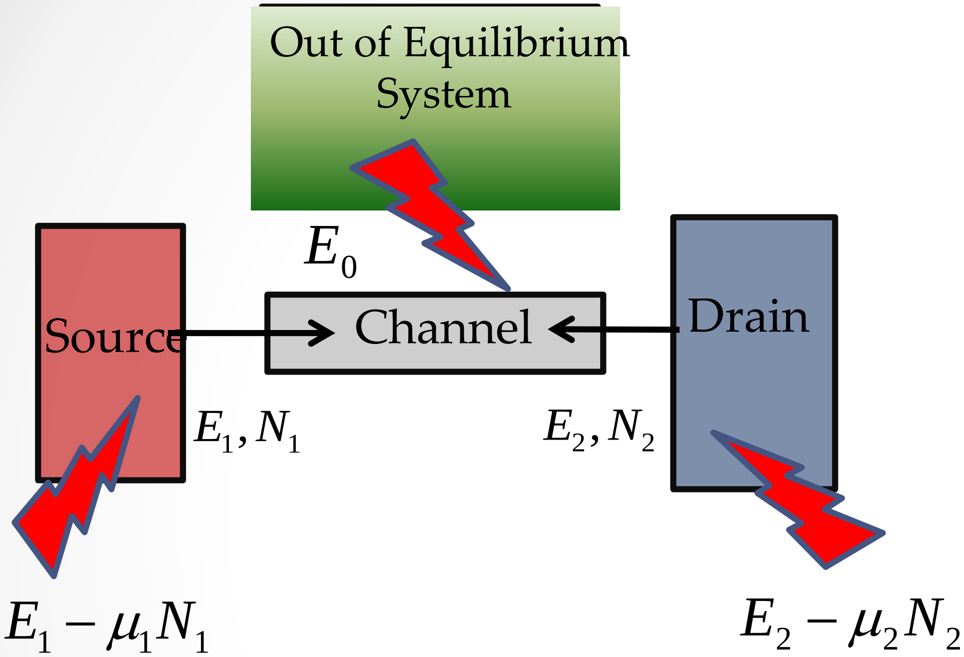
$$R = \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$$

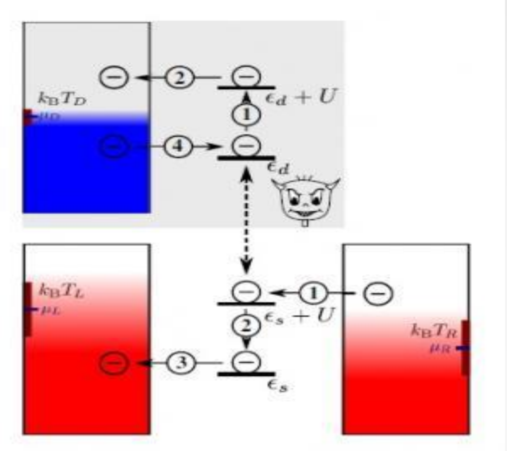
Concurrence Switch

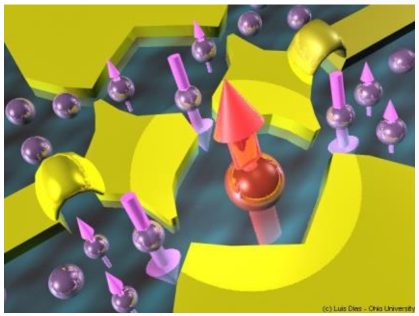


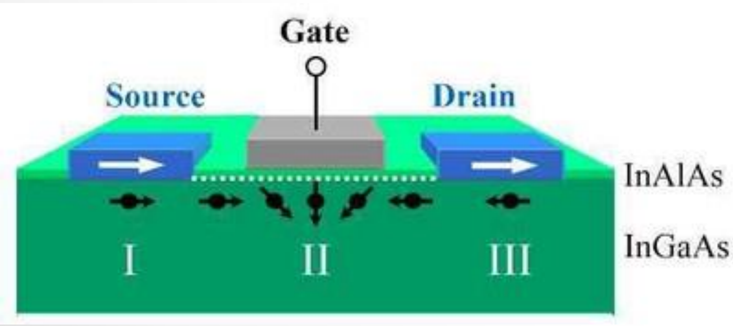


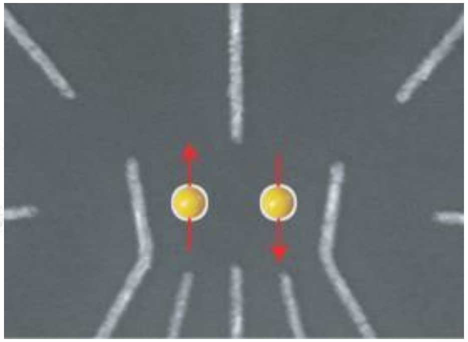
nano-device with “demons”

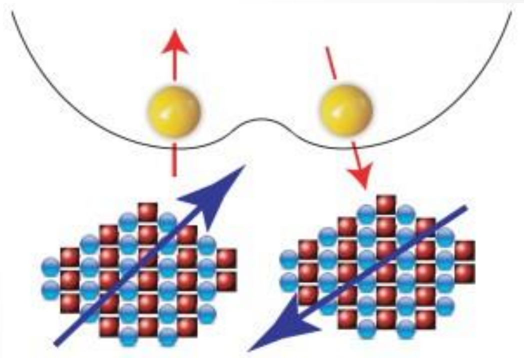




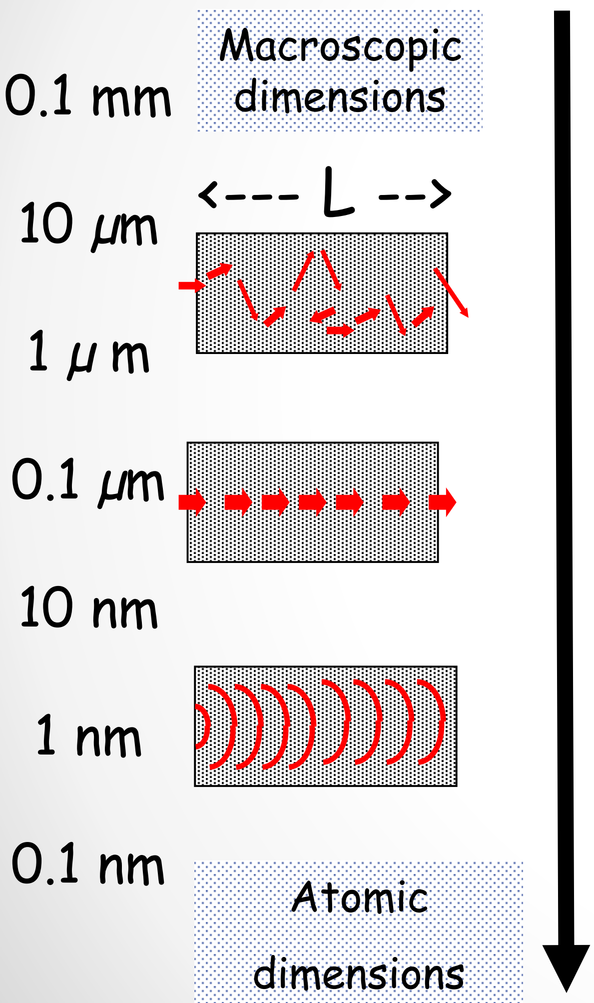


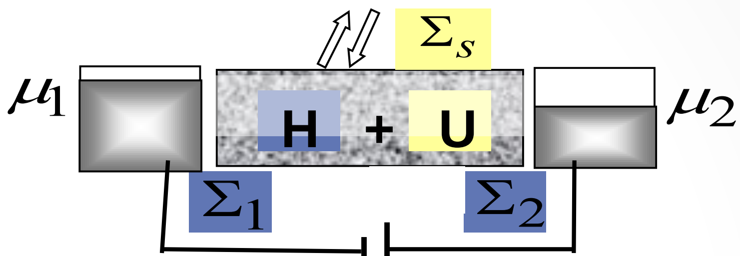






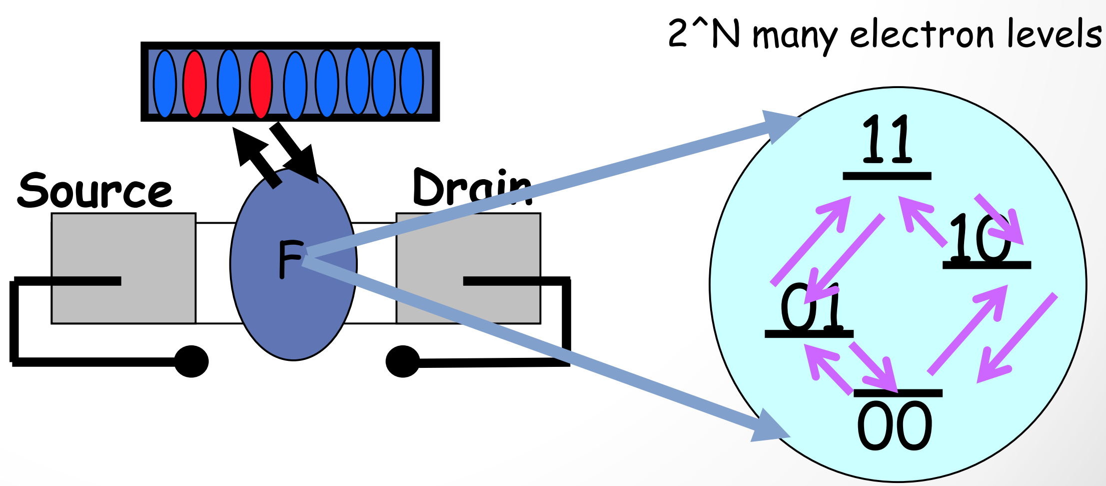
World of Quantum transport



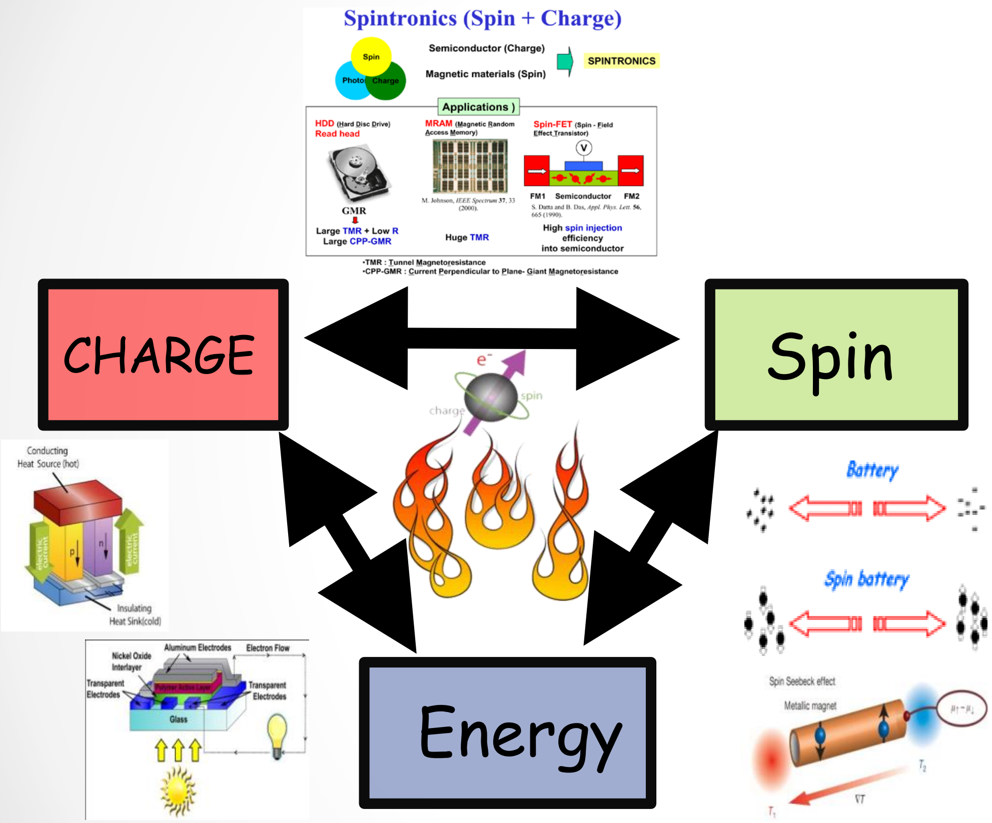


Unified formalism

For quantum transport



Quantum Nano-Energy-Spin Transport



PhD students

- Jyotsna Bahl
- Bitan De
- Debasis Das
- Pankaj Priyadarshi
- Aniket Singha
- Abhishek Sharma
- Swarnadip Mukherjee
- Anirban Basak

Masters/Dual Degree Students

- Arnab Manna
- Aritra Lahiri
- Vivek Arte
- Praveen Sriram

Undergraduate students (B. Tech)

- Varshith Kandula
- Sattwik Deb Mishra
- Sandesh Kalantre
- Abhin Shah