

Sang Wook Kim  
(Pusan N. Univ)



**i**

Information

*heat engine in  
quantum world*

*Kyoto (2015.7.31)*

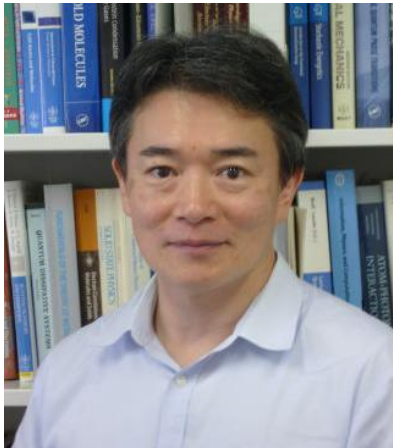
# Collaborators



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# THEORY OF HEAT

BY

J. CLERK MAXWELL, M.A.

LL.D. EDIN., F.R.SS. L. & E.

*Honorary Fellow of Trinity College*

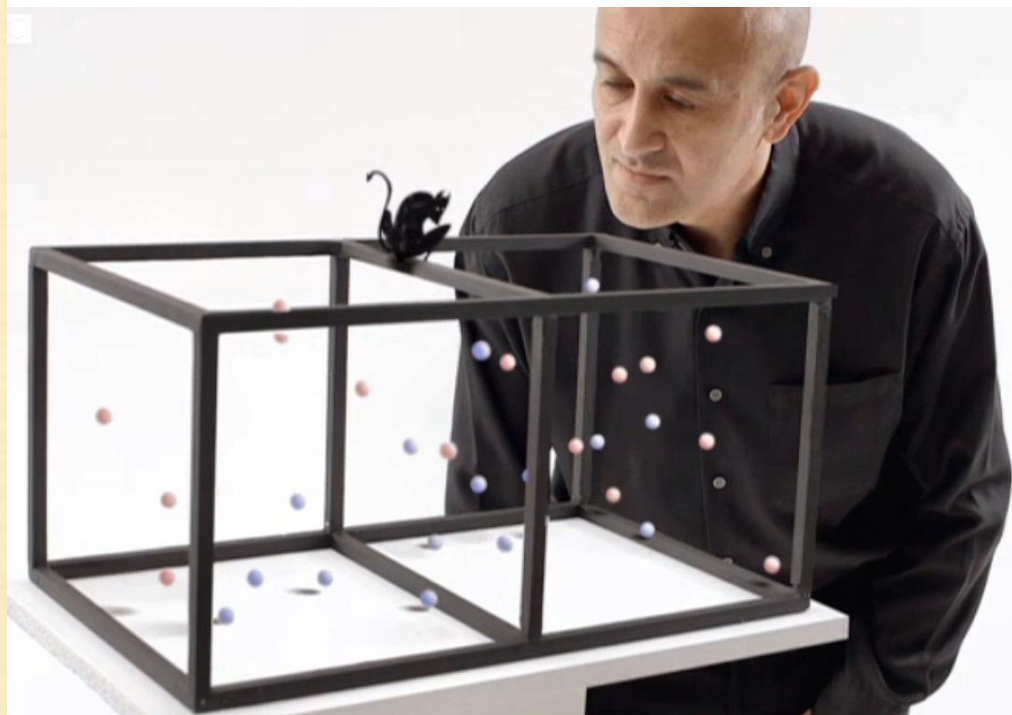
*Professor of Experimental Physics in the University of Cambridge*

Now let us suppose ... that a being, who can see the individual molecules, opens and closes this hole, so as to allow only the swifter molecules to pass from A to B, and only the slower ones to pass from B to A. He will thus, without expenditure of work, raise the temperature of B and lower that of A, in contradiction to the 2<sup>nd</sup> law of thermodynamics.

- J. C. Maxwell (1871)

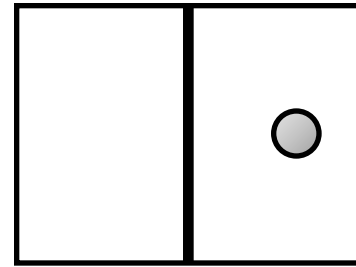
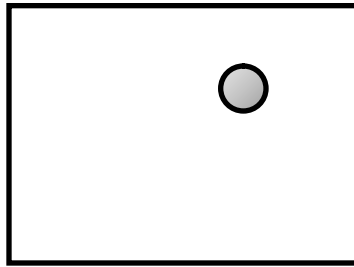
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## Maxwell's Demon

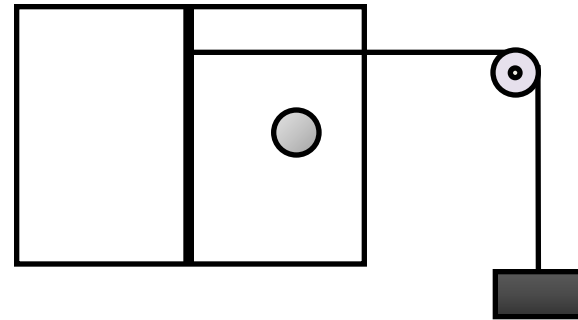
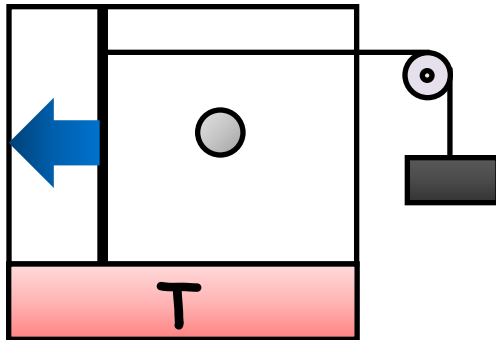




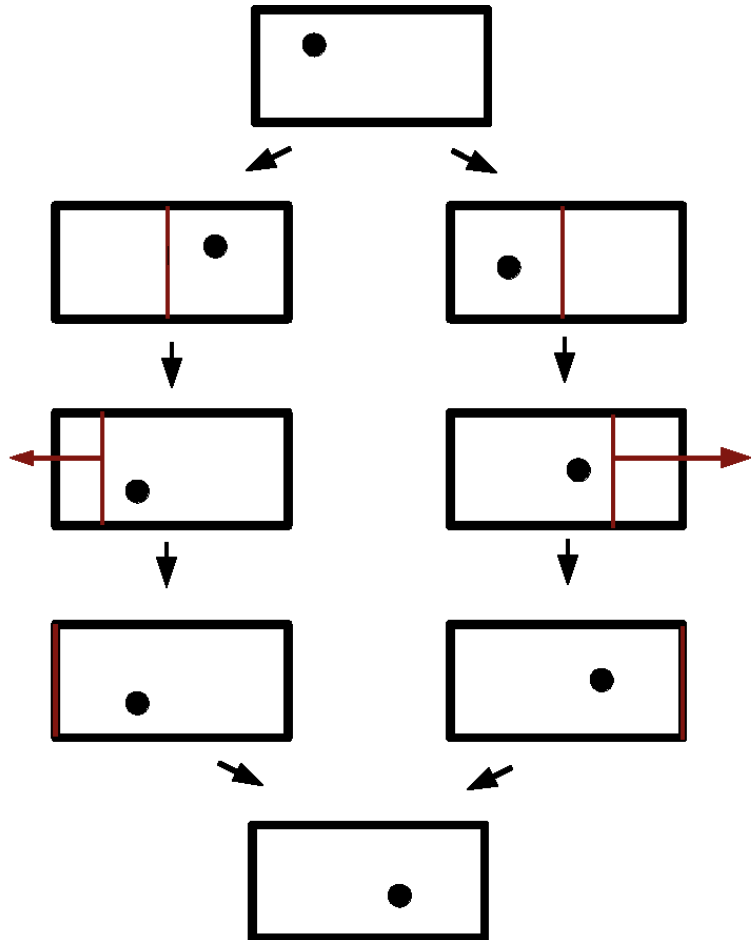
# Szilard's engine (1929)

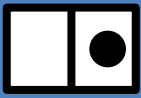




$$W = \int p dV$$



# Flow of entropy

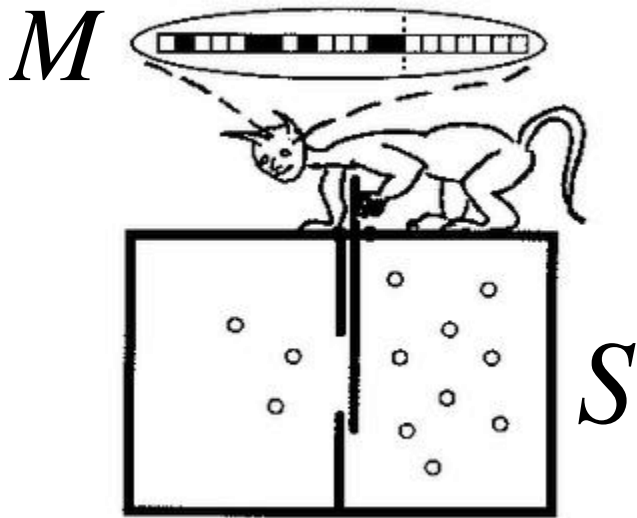


		
$\ln 2$	0	$S_0$
$\ln 2$	$S_0$	
increase	$\ln 2$	decrease
$\ln 2$	$\ln 2$	$S_0 - \ln 2$
$\ln 2$	0	$S_0$

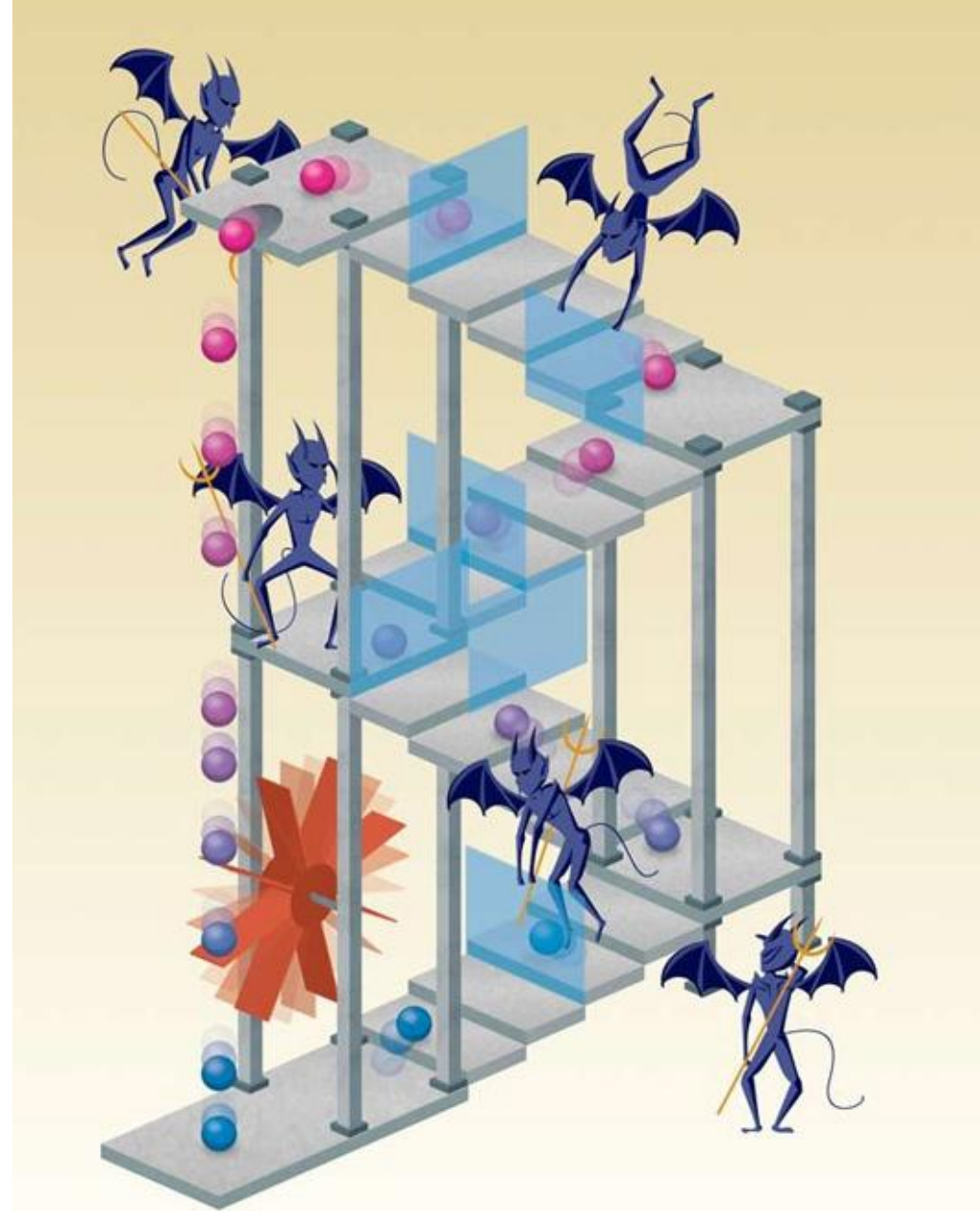
Red arrows indicate the flow of entropy from the first row to the second, from the second to the third, from the third to the fourth, and from the fourth to the fifth.

# Information heat engine

$$W \leq -\Delta F + kT I(S : M)$$



Sagawa & Ueda, PRL (2008)

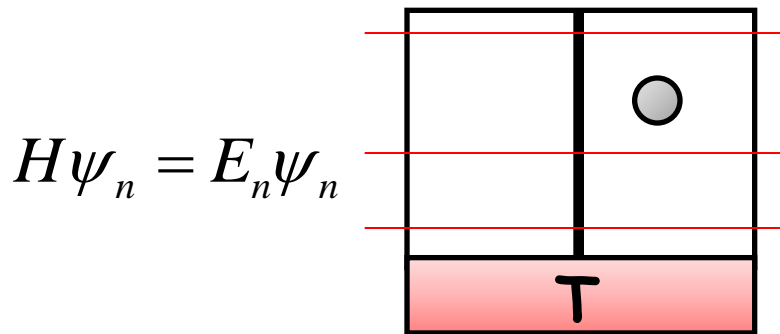


Toyabe, Sagawa, Ueda, Muneyuki & Sano,  
Nature Phys. (2010)

# Quantum dynamical demon?



# Thermodynamic work in Q-world



$$U = \sum_n E_n P_n$$

$$P_n = \frac{e^{-\beta E_n}}{Z} \quad \text{in equilibrium}$$

$Z$   
 ↘  
 partition function

$$dU = \sum_n (E_n dP_n + P_n dE_n)$$

$$\sum_n E_n dP_n = dU - \sum_n P_n dE_n$$

$$TdS = dU + dW$$

$$S = -k \sum_n P_n \ln P_n$$

q-thermodynamic heat

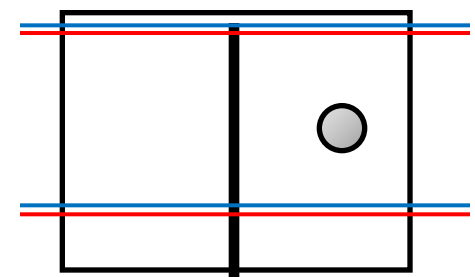
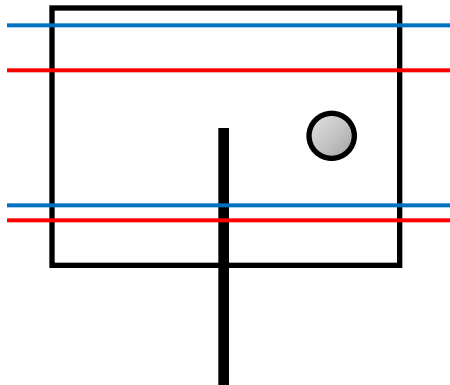
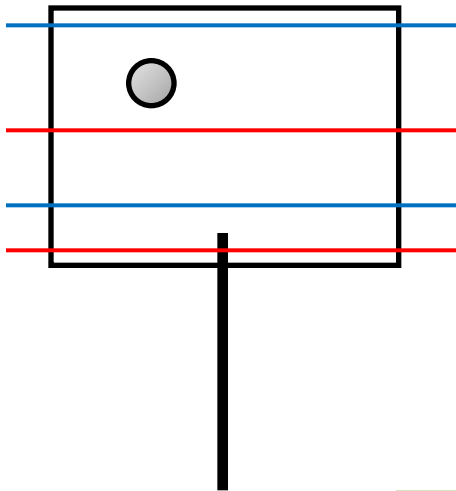
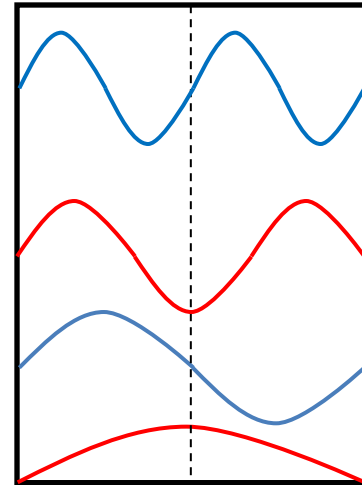
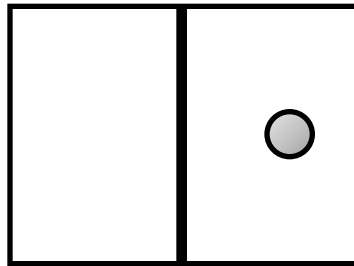
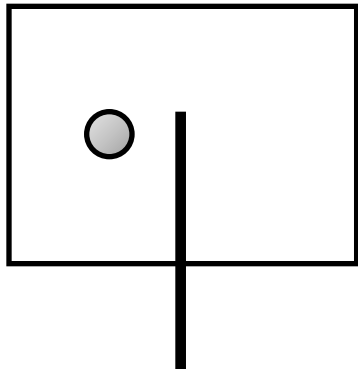
$$dQ = \sum_n E_n dP_n$$

q-thermodynamic work

$$dW = -\sum_n P_n dE_n$$



# Inserting a wall



$$dW = -\sum_n P_n dE_n$$

Inserting a wall is considered as an isothermal process.

# Adiabatic process for inserting a wall

$$dQ = \sum_n E_n dP_n = 0$$

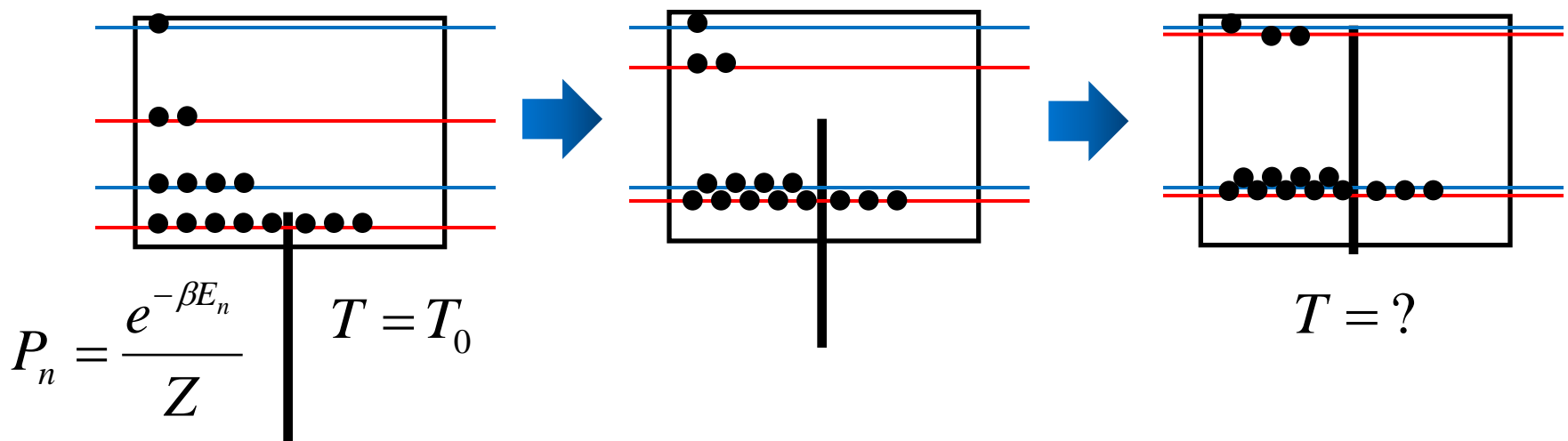
$$dP_n = 0$$

quantum adiabatic

$$dP_n \neq 0$$

$$dQ = \sum_n E_n dP_n = 0$$

T should  
be changed



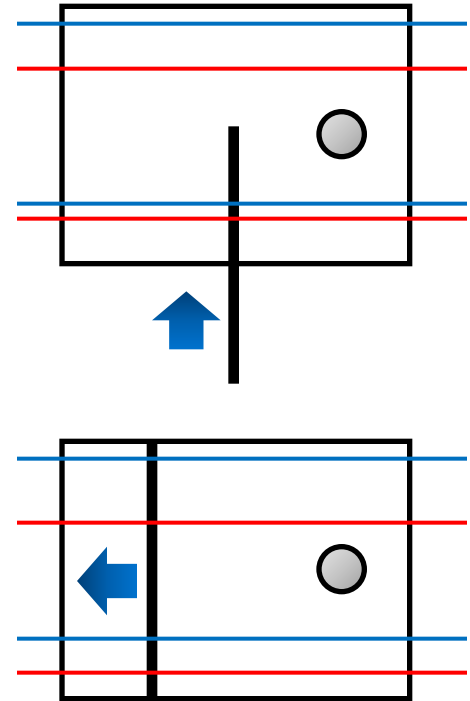
The final state should be in non-equilibrium, so that the irreversible process inevitably occurs in isothermal expansion.

# Q-work in an isothermal process

$$W = -\sum_n \int_{X_1}^{X_2} \frac{e^{-\beta E_n}}{Z} dE_n$$
$$= kT \sum_n \int_{X_1}^{X_2} \frac{\partial \ln Z}{\partial E_n} \frac{\partial E_n}{\partial X} dE$$

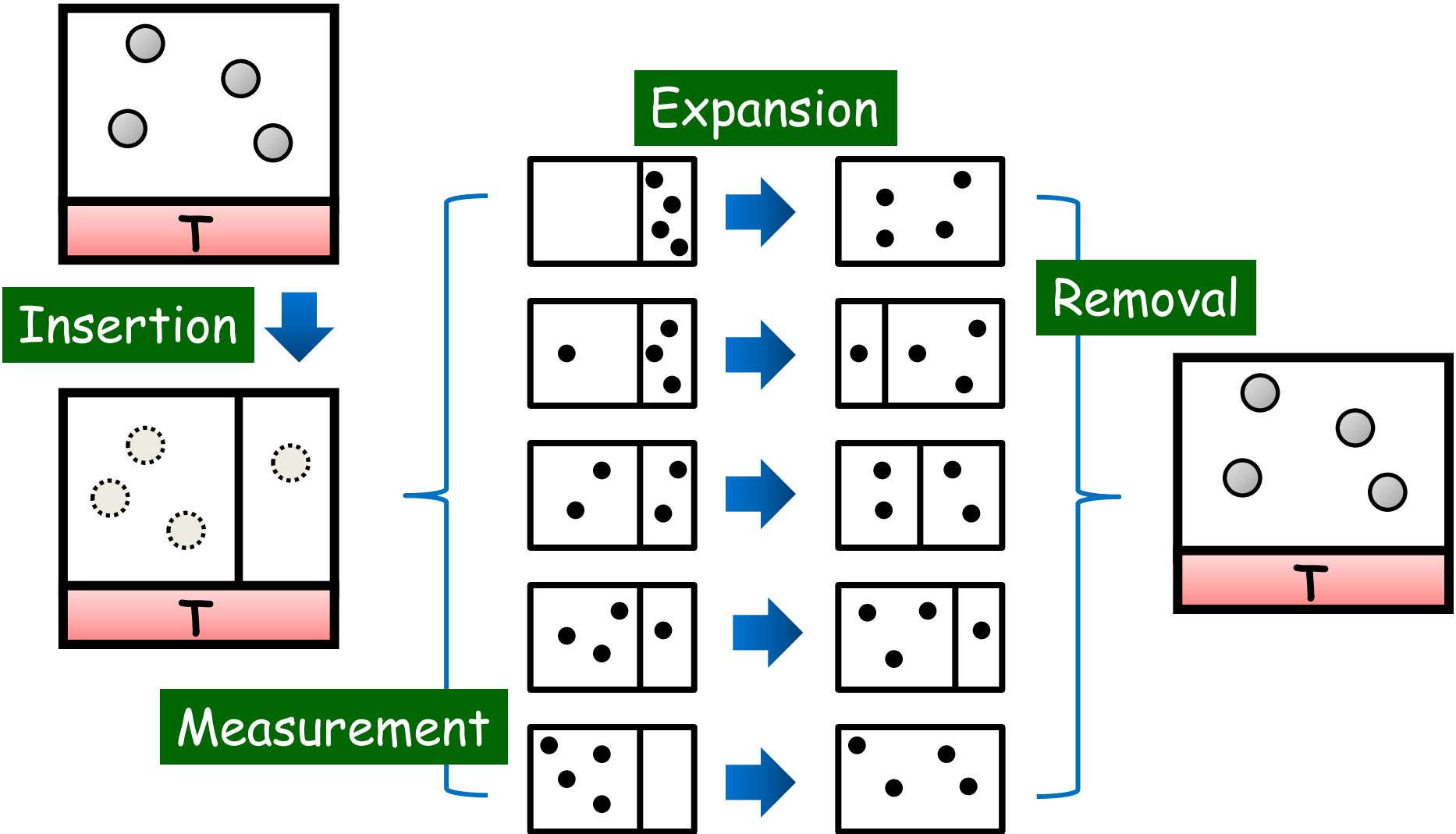
$$= kT [\ln Z(X_2) - \ln Z(X_1)]$$

Helmholtz free energy difference



(Note) Due to isothermal process, we don't have to consider a full density matrix.

# Thermodynamic process



# Q-work of q-Szilard engine

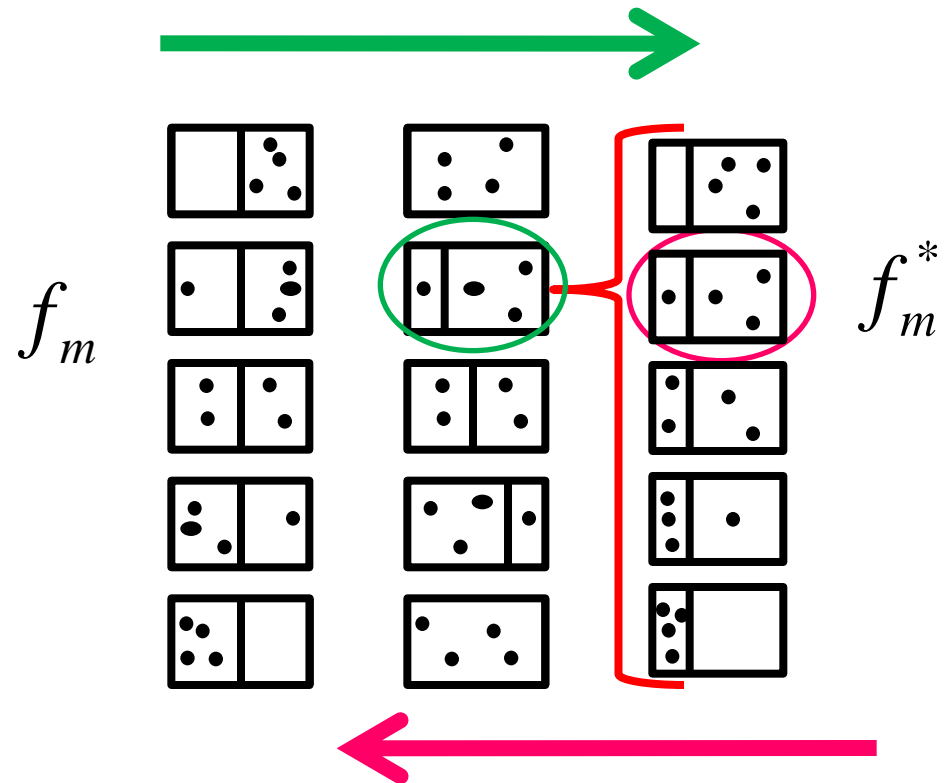
$$W_{tot} = W_{ins} + W_{exp} + W_{rem}$$

$$= -kT \sum_{m=0}^N f_m \ln \left( \frac{f_m}{f_m^*} \right)$$

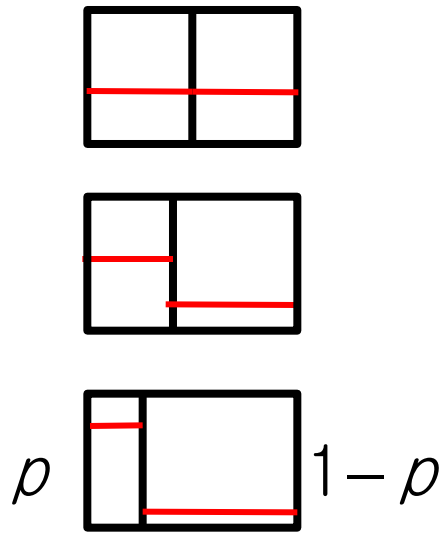
$$f_m^* = \frac{Z_m(l_{eq}^m)}{Z(l_{eq}^m)}$$

$$Z(l_{eq}^m) = \sum_{n=0}^N Z_n(l_{eq}^m)$$

$$\sum_{m=1}^N f_m^* \neq 1$$

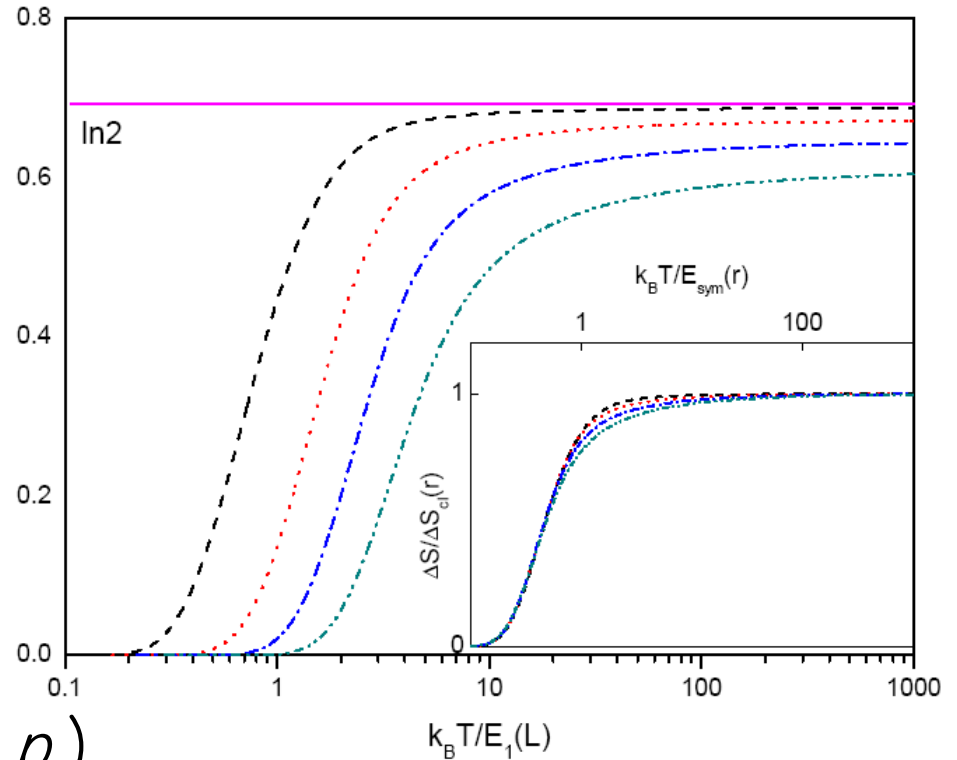


# Single particle $q$ -Szilard engine



$$\frac{W_{tot}}{k_B T}$$

$$\frac{W_{tot}}{k_B T} = -p \ln p - (1-p) \ln(1-p)$$



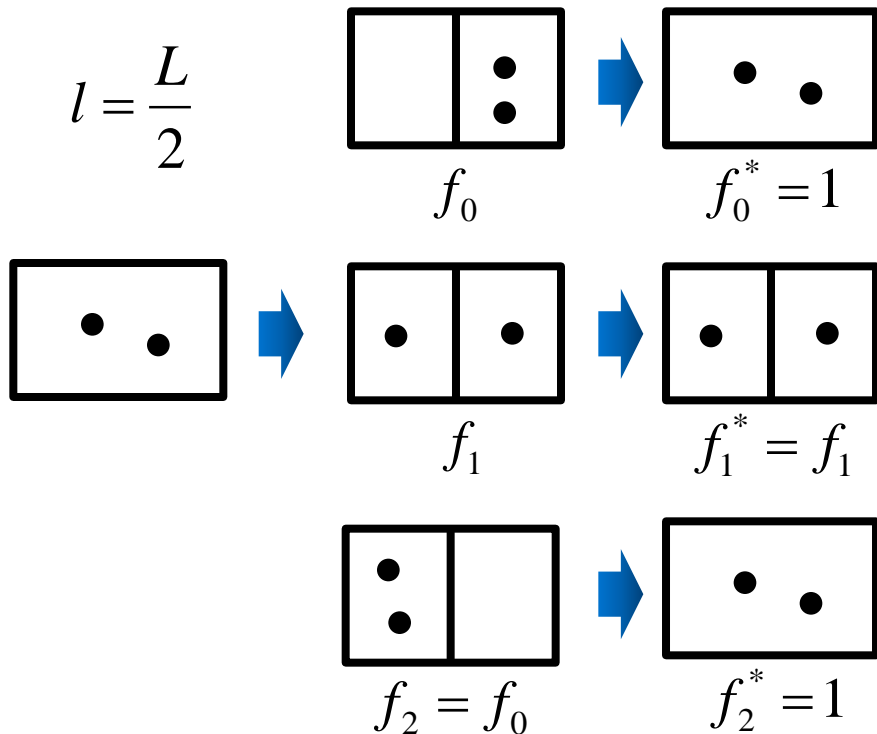
The 3<sup>rd</sup> law of thermodynamics

$$S \rightarrow 0 \text{ as } T \rightarrow 0$$

# Two particle q-Szilard engine I

$$W_{tot} = -kT \sum_{m=0}^N f_m \ln \left( \frac{f_m}{f_m^*} \right)$$

$$W_{tot} = -2kT f_0 \ln f_0$$



$$f_0 = \frac{z^2(l, \beta) + z(l, 2\beta)}{2[2z^2(l, \beta) + z(l, 2\beta)]}$$

$$z(a, b) = \sum_n e^{-bE_n(a)}$$

$$E_n(a) = \frac{h^2}{8m} \frac{n^2}{a^2}$$

# Two particle q-Szilard engine II

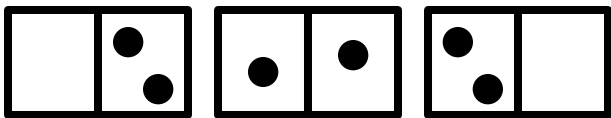
$$W_{tot} = -2kTf_0 \ln f_0$$

Bosons

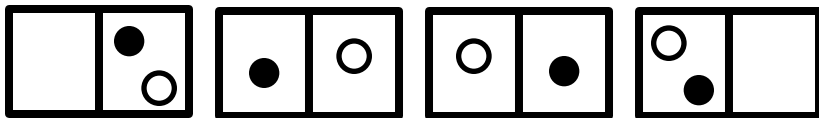
$$W_{tot} \approx kT \left( \frac{2}{3} \right) \ln 3 \quad \text{for } T \rightarrow 0$$

$$W_{tot} \approx kT \ln 2 \quad \text{for } T \rightarrow \infty$$

$$f_0 \rightarrow \frac{1}{3} \quad \text{as } T \rightarrow 0$$



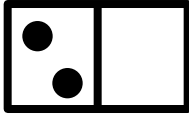
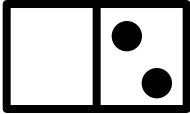
$$f_0 \rightarrow \frac{1}{4} \quad \text{as } T \rightarrow \infty$$



Fermions (spinless)

$$W_{tot} \approx 0 \quad \text{for } T \rightarrow 0$$

$$W_{tot} \approx kT \ln 2 \quad \text{for } T \rightarrow \infty$$

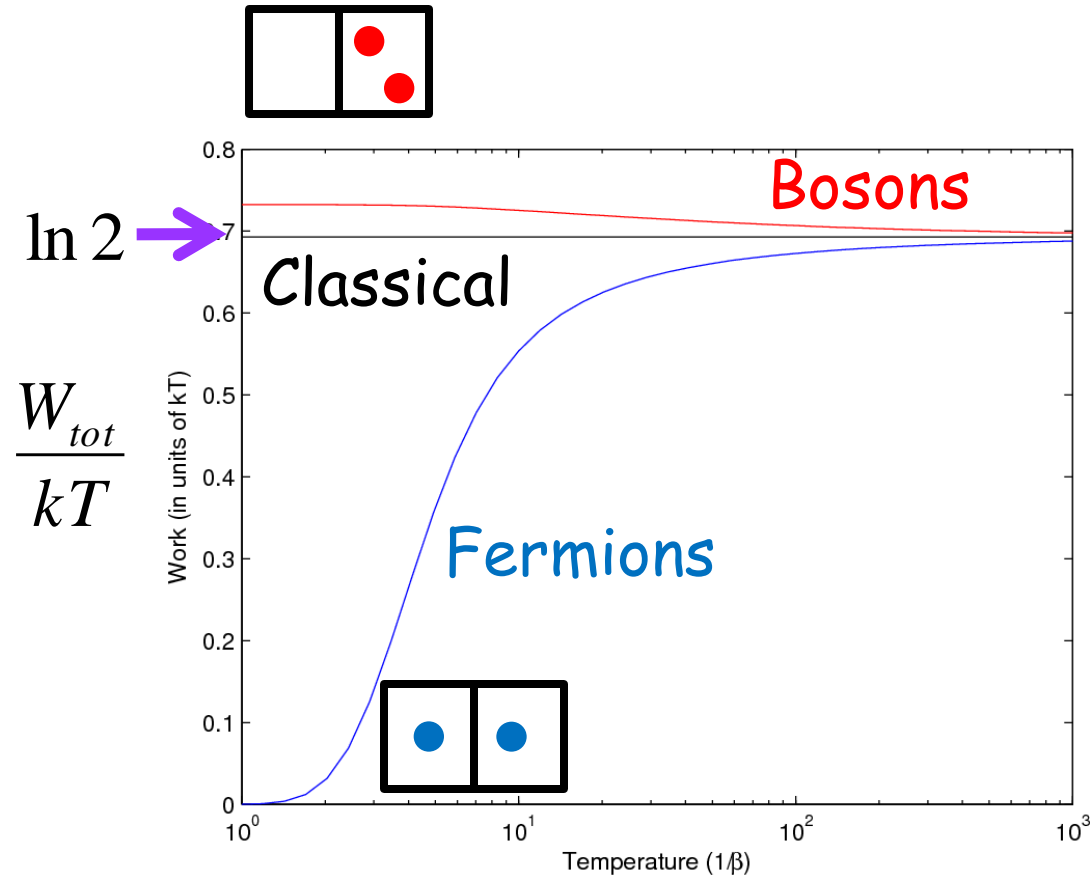
Both  and  are prohibited due to Pauli exclusion principle in the low T.

(cf) classical work

$$W_{classical} = \frac{1}{2} (2kT \ln 2) \quad \img alt="Diagram of one hollow particle in the left box and one solid particle in the right box" data-bbox="851 851 951 928"/>$$



# Two particle q-Szilard engine



APS » Journals » Physics » Viewpoints » Maxwell's demon in the quantum world

## Viewpoint

• Statistical Mechanics • Quantum Information

Physics 4, 13 (2011)

DOI: 10.1103/Physics.4.13

## Maxwell's demon in the quantum world

Juan M. R. Parrondo and Jordan M. Horowitz

Departamento de Física Atómica, Molecular y Nuclear and GISC, Universidad Complutense de Madrid, 28040-Madrid, Spain

Published February 14, 2011

Extraction of work from a heat bath using the Szilard engine depends crucially on the statistics of indistinguishable particles.

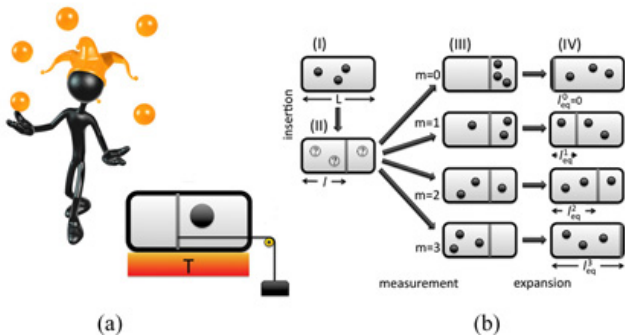
### A Viewpoint on:

#### Quantum Szilard Engine

Sang Wook Kim, Takahiro Sagawa, Simone De Liberato, and Masahito Ueda

Phys. Rev. Lett. **106**, 070401 (2011) – Published February 14, 2011

[Download PDF \(free\)](#)



Information and thermodynamics are intimately connected. This idea was first illustrated by Maxwell with his celebrated demon: an intelligent being who uses his knowledge about the position and velocity of the molecules in a gas to transfer heat against a temperature gradient without expenditure of work, beating the second law of thermodynamics. The Szilard engine is a stylized version of the demon, where a yes/no measurement of a classical single-particle system allows one to extract a tiny amount of energy,  $kT \ln 2$ ,  $k$  being the Boltzmann constant, from a thermal reservoir at temperature  $T$ . The engine has been around for almost a century now [1]. Along the way it has furnished insight into the foundations of statistical mechanics, become the canonical model for investigations of feedback-controlled systems, and even spurred the creation of a new field: the thermodynamics of

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**Phys. Rev. Lett. 111, 188901 (2013) [1 pages]**

## Comment on “Quantur

Abstract

References

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Martin Plesch<sup>1,2</sup>, Oscar Dahlsten<sup>3,4</sup>, John Gool

<sup>1</sup>Faculty of Informatics, Masaryk University, Brn

<sup>2</sup>Institute of Physics, Slovak Academy of Scienc

<sup>3</sup>Department of Physics, University of Oxford, C

<sup>4</sup>Center for Quantum Technology, National Uni

Received 22 November 2012; published 30 Oc

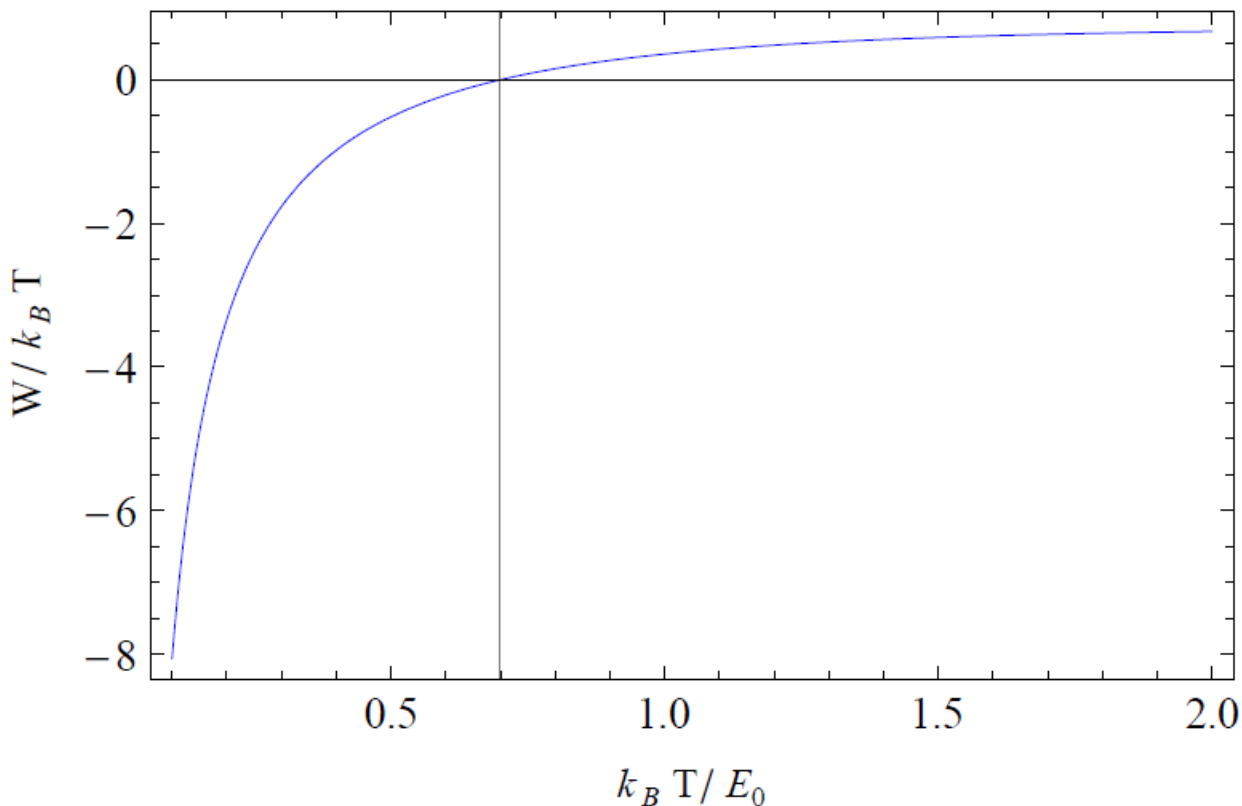
A Comment on the Letter by S. W. Kim *et al.*, Ph

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URL: <http://link.aps.org/doi/10.1103/PhysRevL>

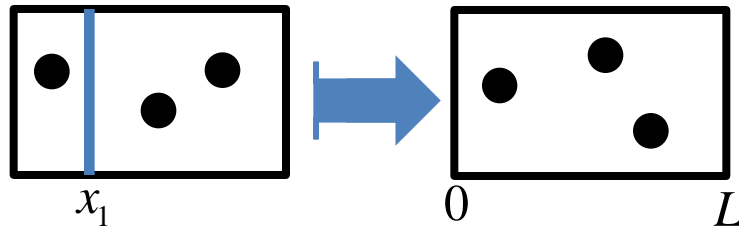
DOI: 10.1103/PhysRevLett.111.188901

PACS: 05.30.-d, 03.67.-a, 05.70.-a, 89.70.Cf

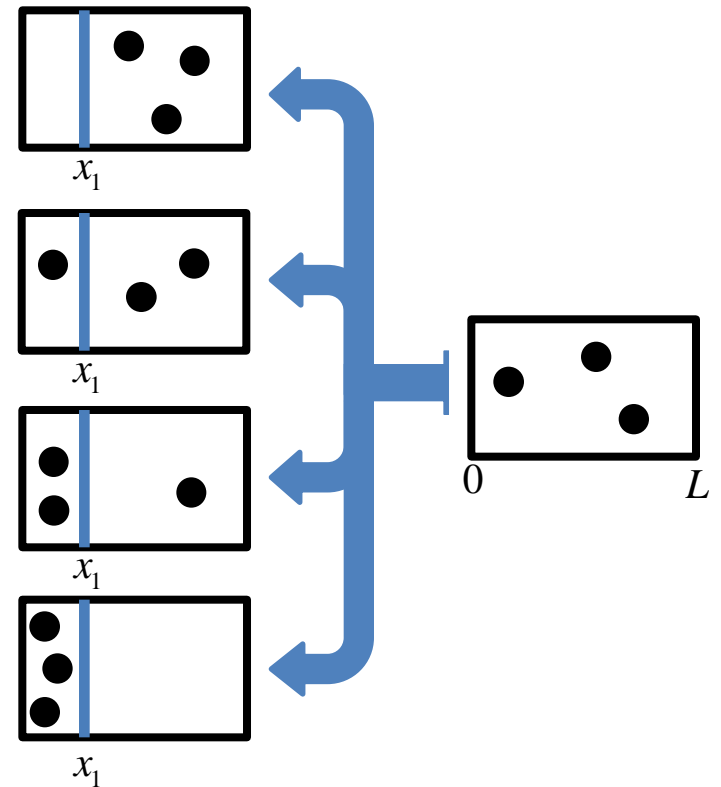


# Irreversible process I

Time-forward



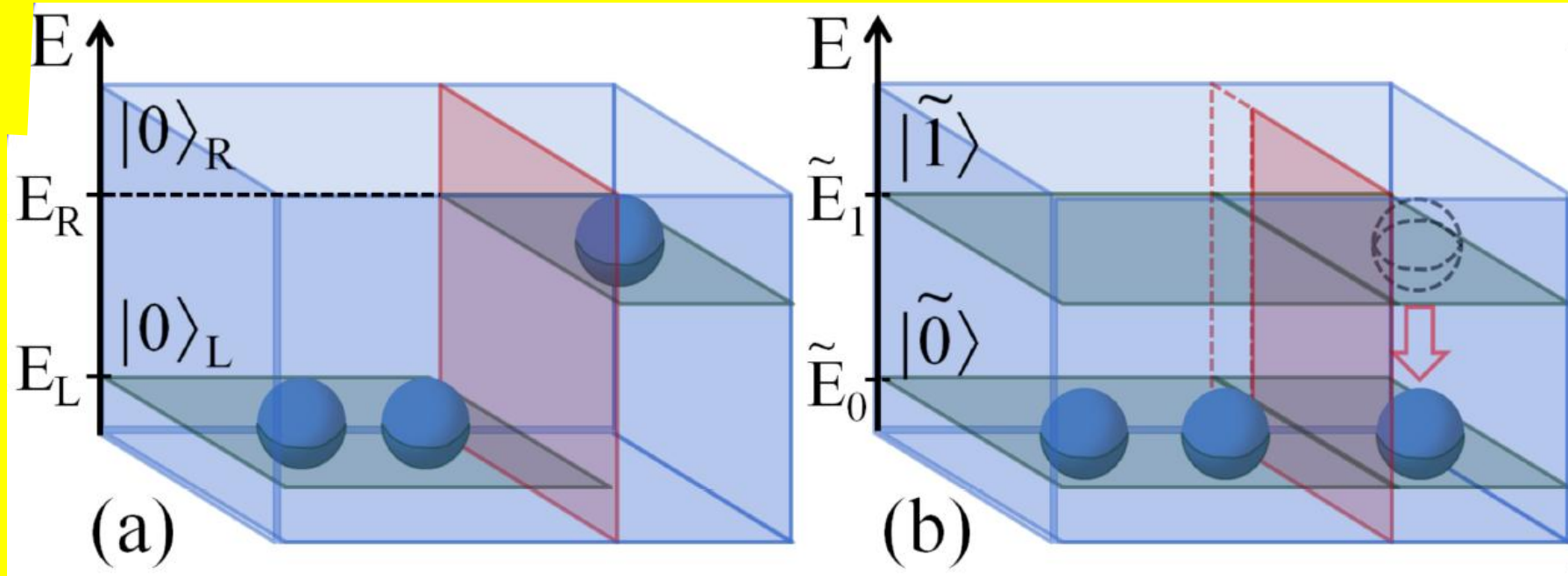
Time-backward



**Inherently  
irreversible!**

(cf) Murashita, Funo & Ueda, PRE (2014)  
Ashida, Funo, Murashita & Ueda, PRE (2014)

# Irreversible process II

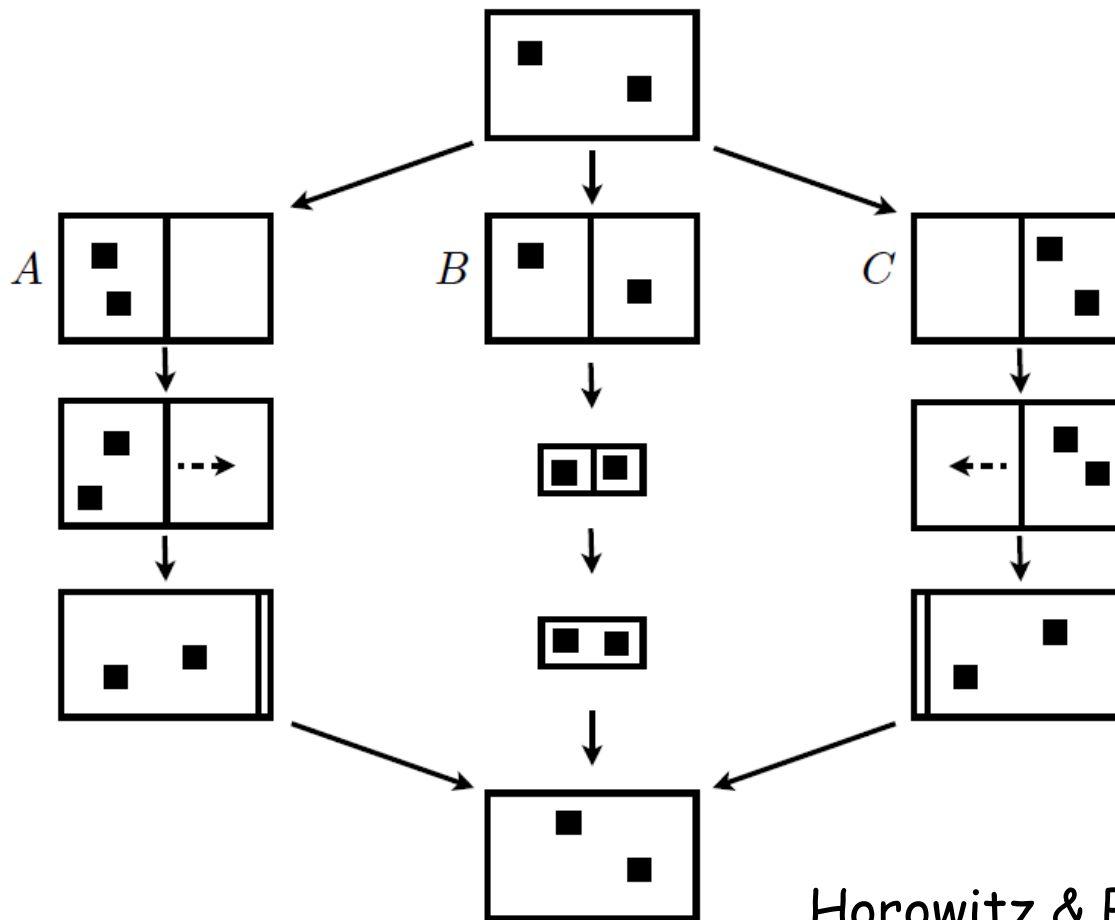


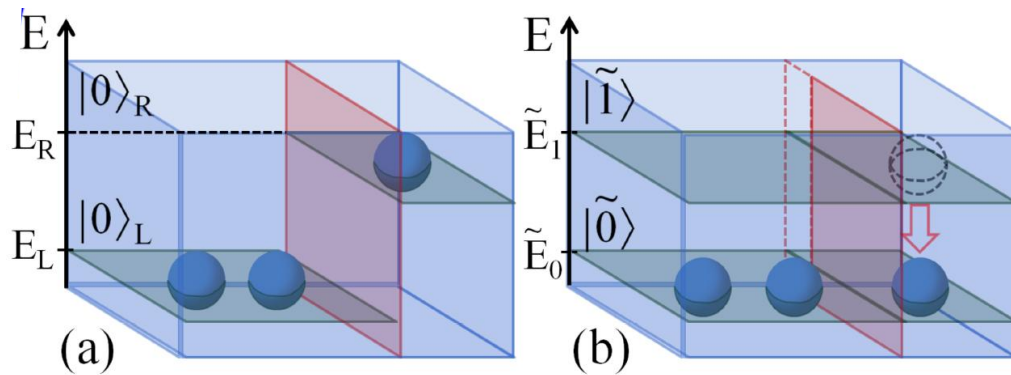
$T$

$$W_{tot} = kT \left\{ - \sum_{m=0}^N f_m \ln f_m + \left( - \sum_{m=0}^N f_m \ln f_m^* \right) \right\}$$

# (Option 1)

## Make the protocol reversible





## (Option 2) Optimize work via math

$$W_{tot} = -kT \sum_{m=0}^N f_m \ln \left( \frac{f_m}{f_m^*} \right)$$

$$W_{tot}(l, \{x_m\})$$

Optimal condition:

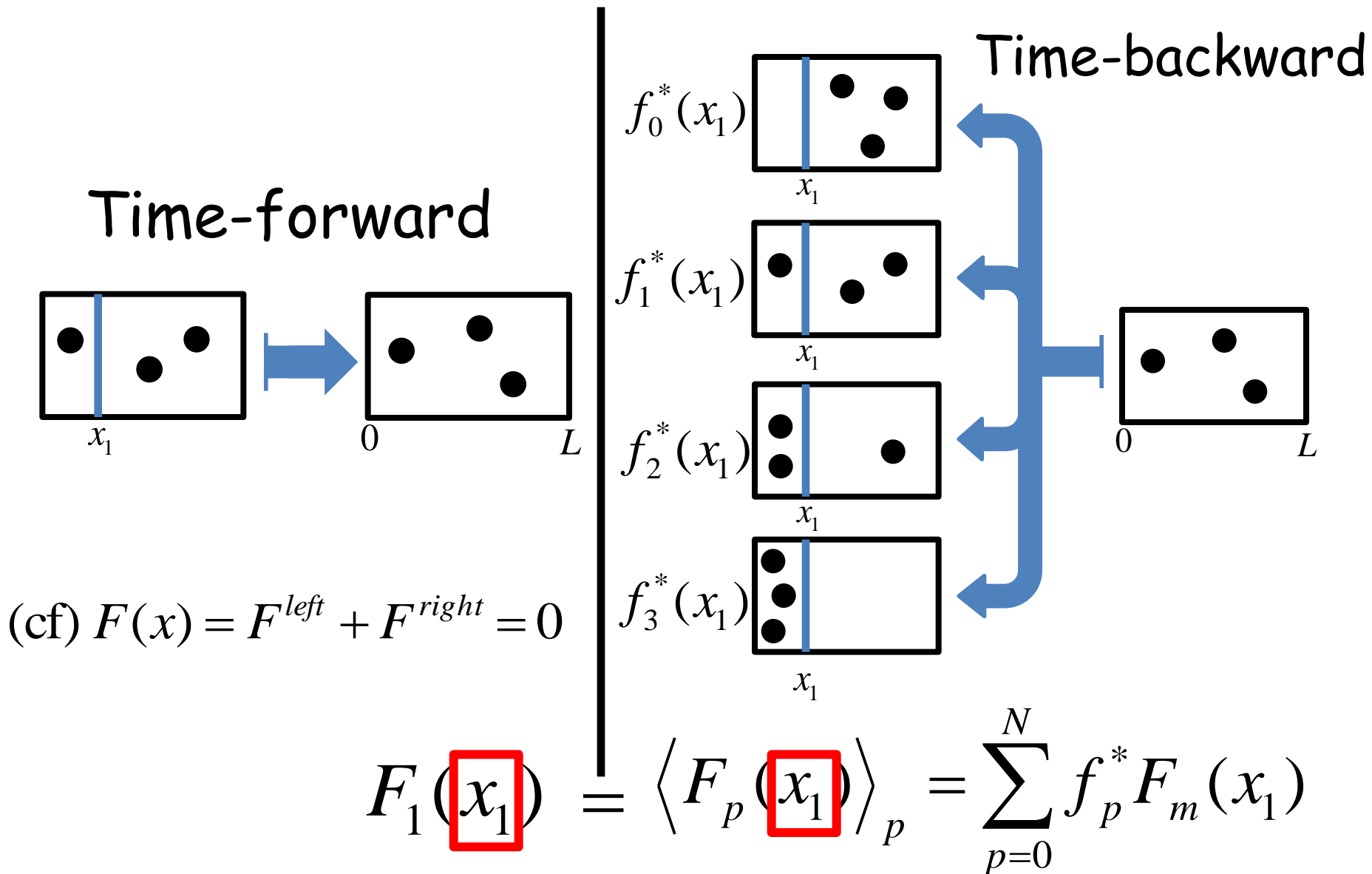
$$\nabla_{l, x_m} W_{tot}(l, \{x_m\}) = 0$$

$$\frac{1}{Z_m} \frac{\partial Z_m}{\partial x_m} = \frac{1}{Z} \frac{\partial Z}{\partial x_m}$$

$$F_m(x_m) = \langle F_p(x_m) \rangle_p$$

$$W_{tot} \geq 0$$

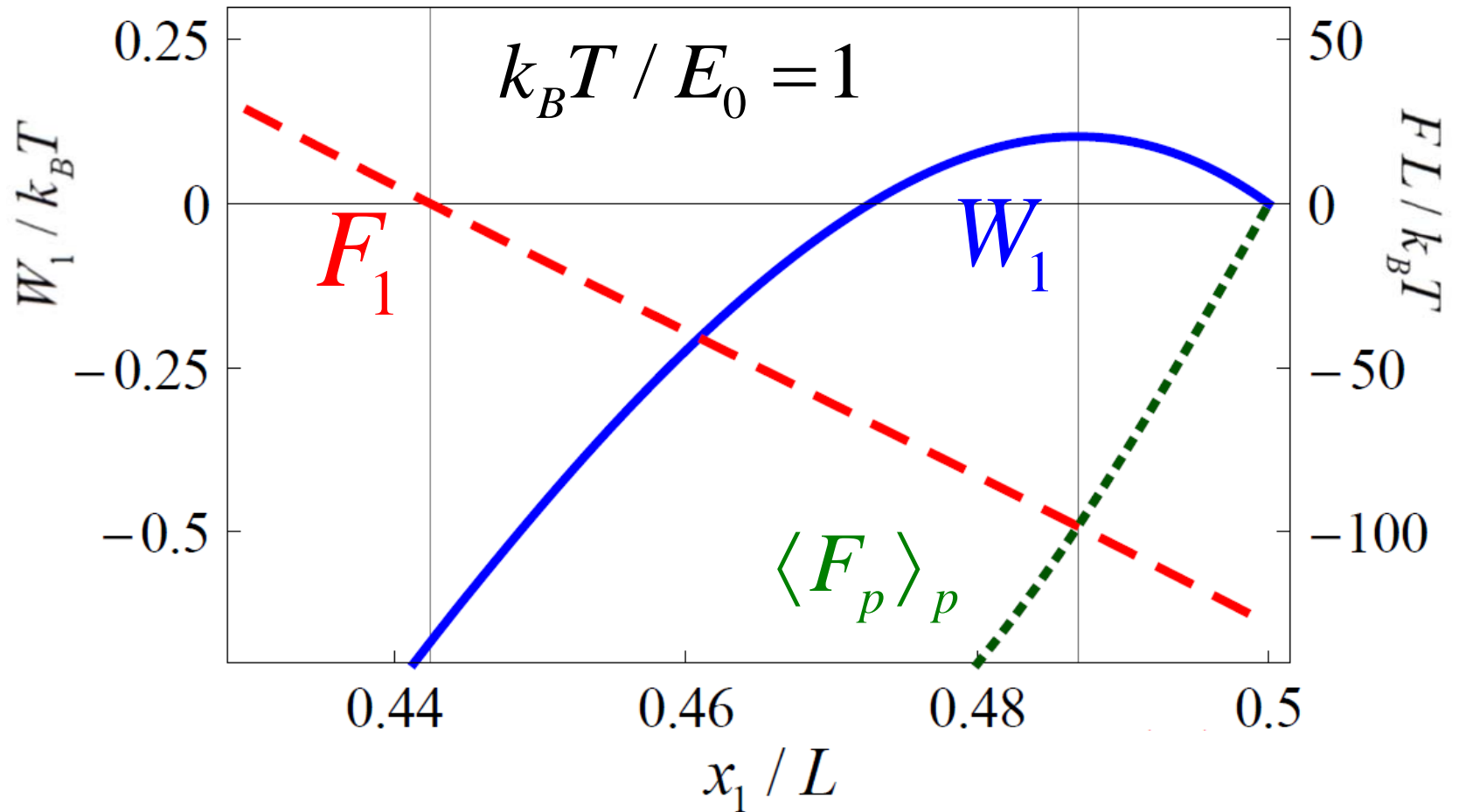
# Physical meaning of optimal condition



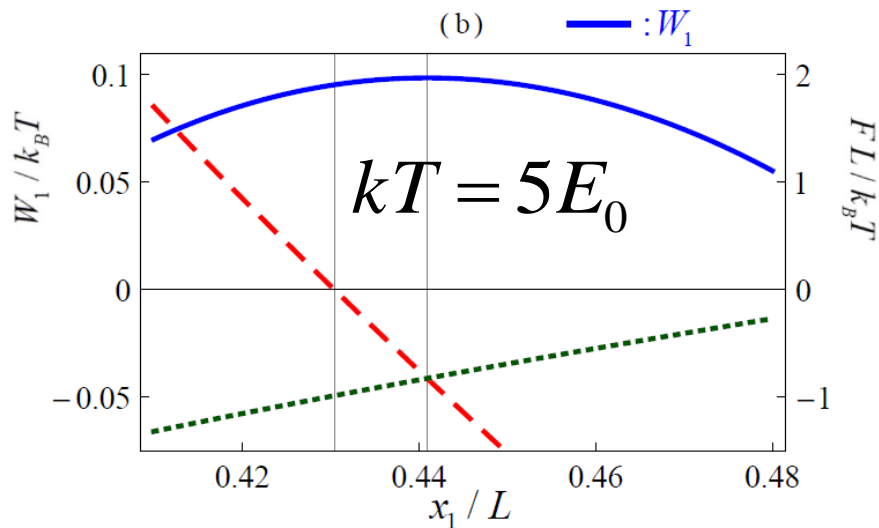
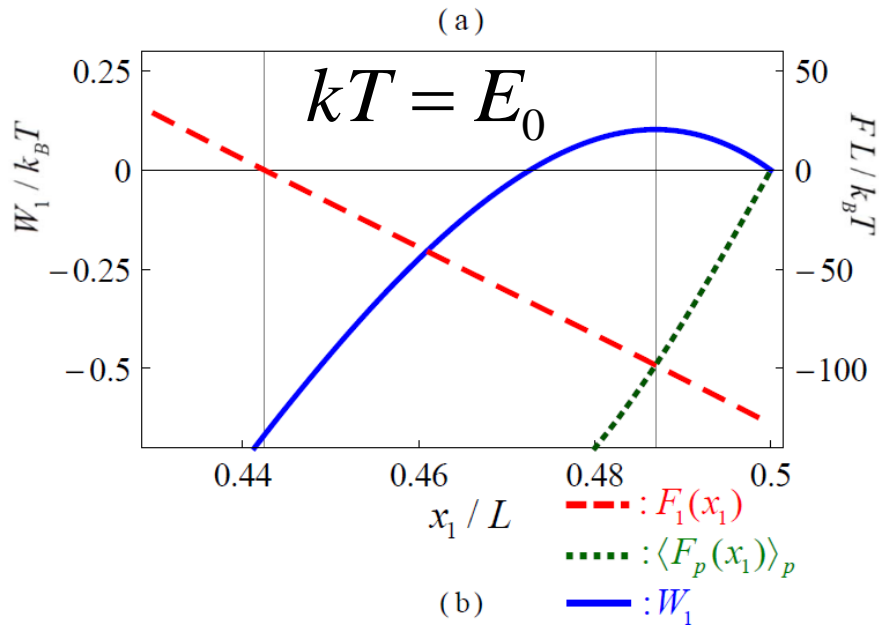


# Numerical check I

*Boson*  $N = 3$



# Numerical check II



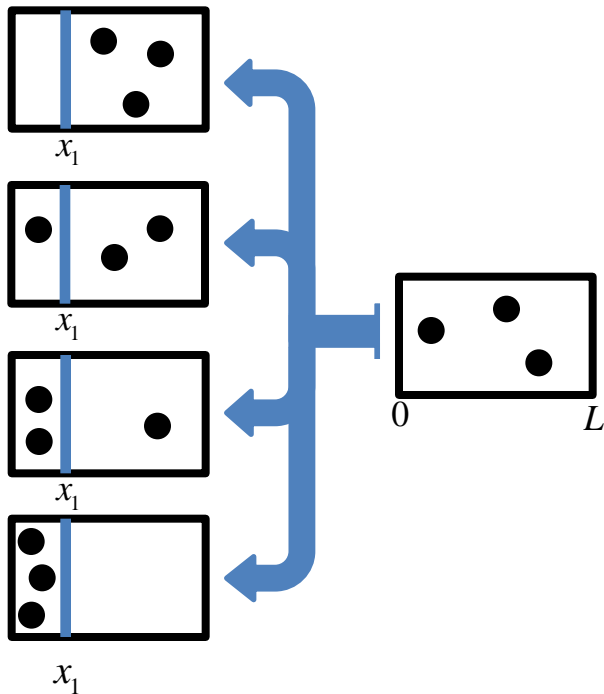
$$\langle F_p(x_1) \rangle_p \rightarrow 0$$

$$T \rightarrow \infty$$

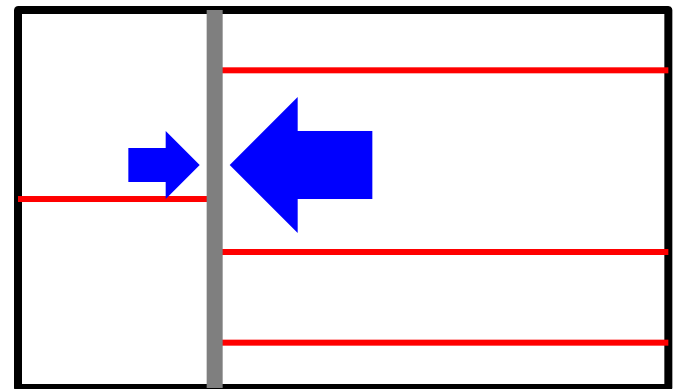
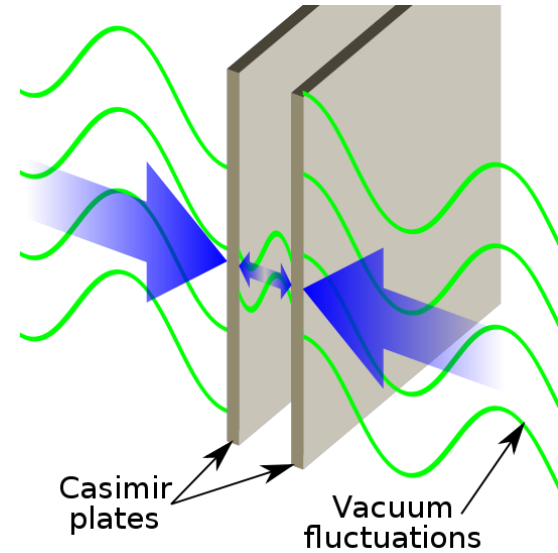
$$\langle F_p(x_1) \rangle_p = \sum_{p=0}^N f_p^* F_m(x_1) \neq 0$$

Why?

Time-backward

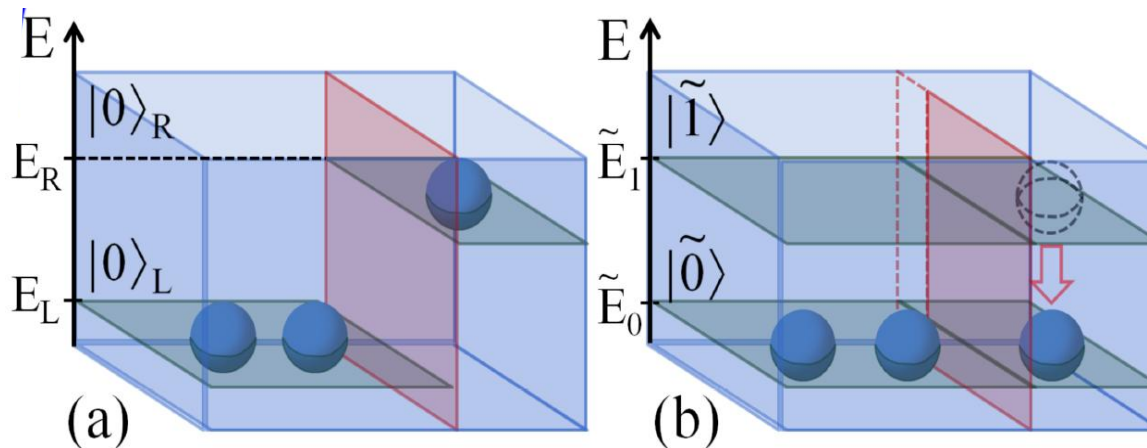


# Casimir force



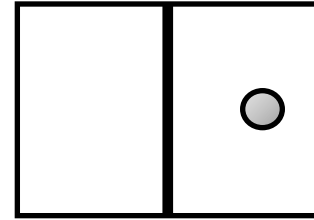
The optimal condition of the  $q$ -SZE with intrinsic irreversibility is achieved once the time-forward force is equivalent to the time back-ward force:

$$F_m(x_m) = \langle F_p(x_m) \rangle_p$$



# Remark and a new question

$$W_{tot} = -kT \sum_{m=0}^N f_m \ln \left( \frac{f_m}{f_m^*} \right)$$



In fact, this equation can be derived from fully **classical** consideration. The point is that the above expression is mainly ascribed to multi-particle nature of SZE.

Is work extractable from a heat engine by using purely quantum mechanical information? If yes, what is its mathematical formula?

# Quantum information demon?



- Previous works

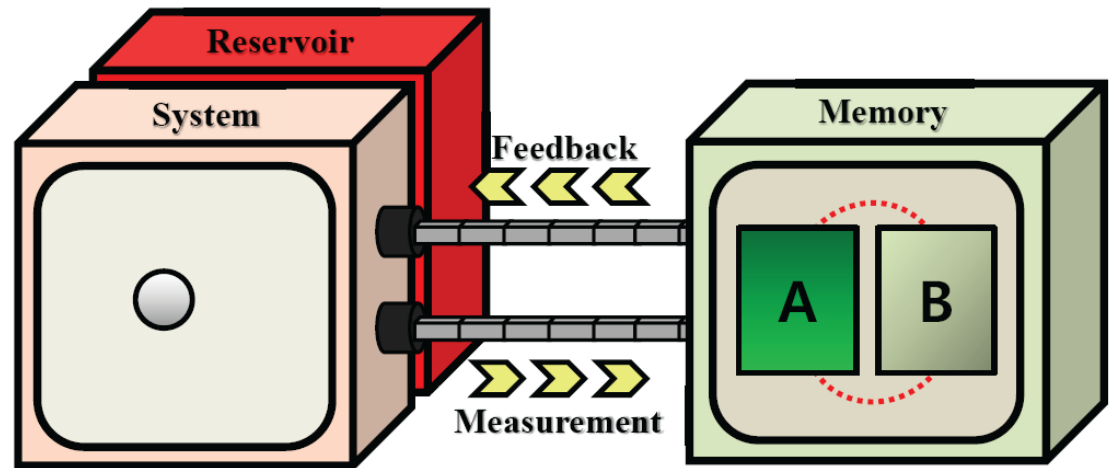
Oppenheim, Horodecki, Horodecki & Horodecki, PRL (2002)

Zurek, PRA (2003)

Rio, Aberg, Renner, Dahlsten & Vedral, Nature (2011)

Funo, Watanabe & Ueda, PRA (2013)

# Our Set-up



$$\rho^{(i)} = \rho_{AB}^{(i)} \otimes \frac{\exp(-\beta H_S^{(i)})}{Z_S^{(i)}} \otimes \frac{\exp(-\beta H_R^{(i)})}{Z_R^{(i)}}$$

Park, K.-H. Kim, Sagawa & SWK, PRL (2013)

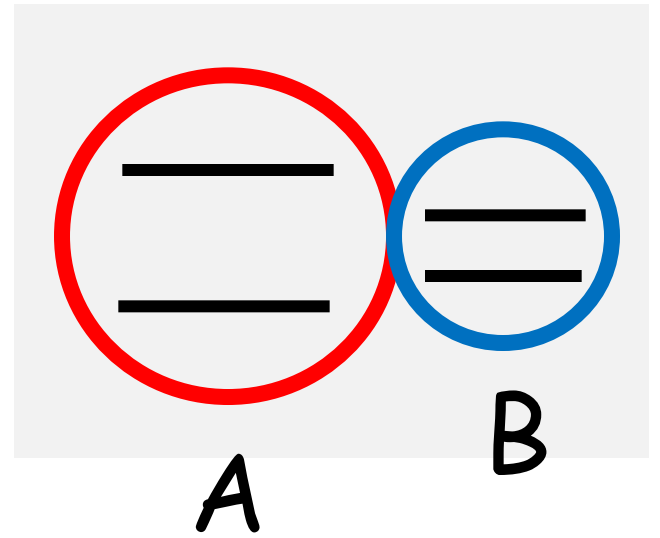
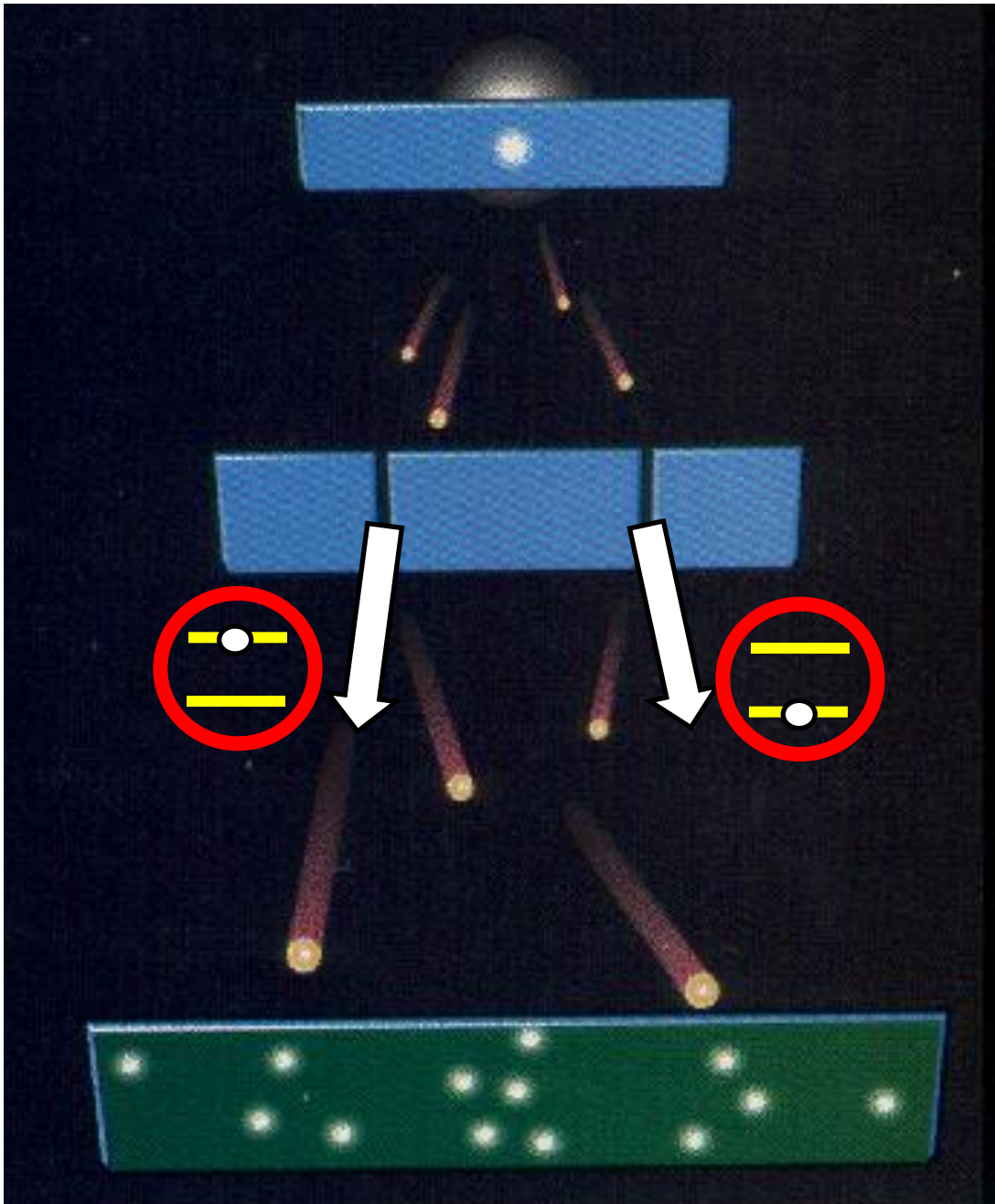
# Origin of quantum-mechanical complementarity probed by a 'which-way' experiment in an atom interferometer

S. Dürr, T. Nonn & G. Rempe

*Fakultät für Physik, Universität Konstanz, 78457 Konstanz, Germany*

**The principle of complementarity refers to the ability of quantum-mechanical entities to behave as particles or waves under different experimental conditions. For example, in the famous double-slit experiment, a single electron can apparently pass through both apertures simultaneously, forming an interference pattern. But if a 'which-way' detector is employed to determine the particle's path, the interference pattern is destroyed. This is usually explained in terms of Heisenberg's uncertainty principle, in which the acquisition of spatial information increases the uncertainty in the particle's momentum, thus destroying the interference. Here we report a which-way experiment in an atom interferometer in which the 'back action' of path detection on the atom's momentum is too small to explain the disappearance of the interference pattern. We attribute it instead to correlations between the which-way detector and the atomic motion, rather than to the uncertainty principle.**





# Thermodynamic process

Stage 1 (unitary evolution)

$$\rho^{(1)} = U^{(1)} \rho^{(i)} U^{(1)\dagger} \quad U^{(1)} = I_{AB} \otimes U_{SR}^{(1)}$$

This can also describe isothermal process.

Stage 2 (POVM)

$$\rho^{(2)} = \sum_k \Pi_A^k U^{(2)} \rho^{(1)} U^{(2)\dagger} \Pi_A^k = \sum_k p_k |k\rangle_A \langle k| \otimes \rho_{BSR}^{(2)k}$$

$$p_k \equiv \text{tr}[\Pi_A^k U^{(2)} \rho^{(1)} U^{(2)\dagger} \Pi_A^k] \quad \rho_{BSR}^{(2)k} \equiv \text{tr}_A[\Pi_A^k U^{(2)} \rho^{(1)} U^{(2)\dagger} \Pi_A^k]$$

Stage 3 (feedback control)

$$\rho^{(f)} = U^{(3)} \rho^{(2)} U^{(3)\dagger}$$

# Entropy consideration

von Neumann entropy  $S(\rho) \equiv -\text{tr}(\rho \ln \rho)$

(1) concavity 
$$\sum_k p_k S[\rho_{SR}^{(2)k}] \leq S[\rho_{SR}^{(f)}]$$

(2) POVM 
$$S[\rho^{(i)}] \leq S[\rho^{(2)}]$$

(3) Klein inequality 
$$\text{tr}[\rho_{SR}^{(f)} \ln \rho_{SR}^{(f)\text{can}}] \leq S[\rho_{SR}^{(f)}]$$

$$W \leq -\Delta F_S + kT(\Delta S_A + \Delta S_B) - kT\Delta I$$

$$\Delta I \equiv I(A^{(2)} : B^{(2)}) - I(A^{(i)} : B^{(i)})$$

mutual information  $I(A : B) \equiv S(\rho_A) + S(\rho_B) - S(\rho_{AB}) = I(B : A)$

Park, K.-H. Kim, Sagawa & SWK, PRL (2013)

# Mutual information and Discord

classical mutual information

$$J(B : A) \equiv H(B) + H(A) - H(B, A) = H(B) - H(B | A)$$

Shanon information  $H(A) \equiv -\sum_A p(A) \ln p(A)$

conditional entropy  $H(B | A) \equiv -\sum_{A,B} p(A, B) \ln p(B | A)$

quantum analogue

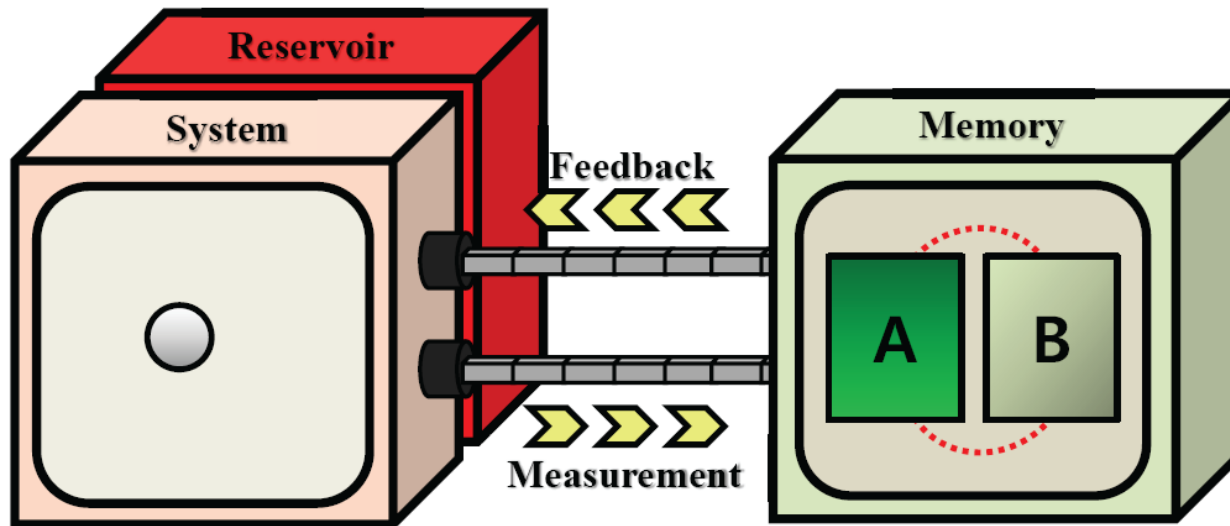
$$\tilde{J}(B : A) = S(B) - S(B | A) ???$$

$$\tilde{J}_{\{\Pi_A^i\}}(B : A) = S(\rho_B) - S(\rho_B | \{\Pi_A^i\})$$

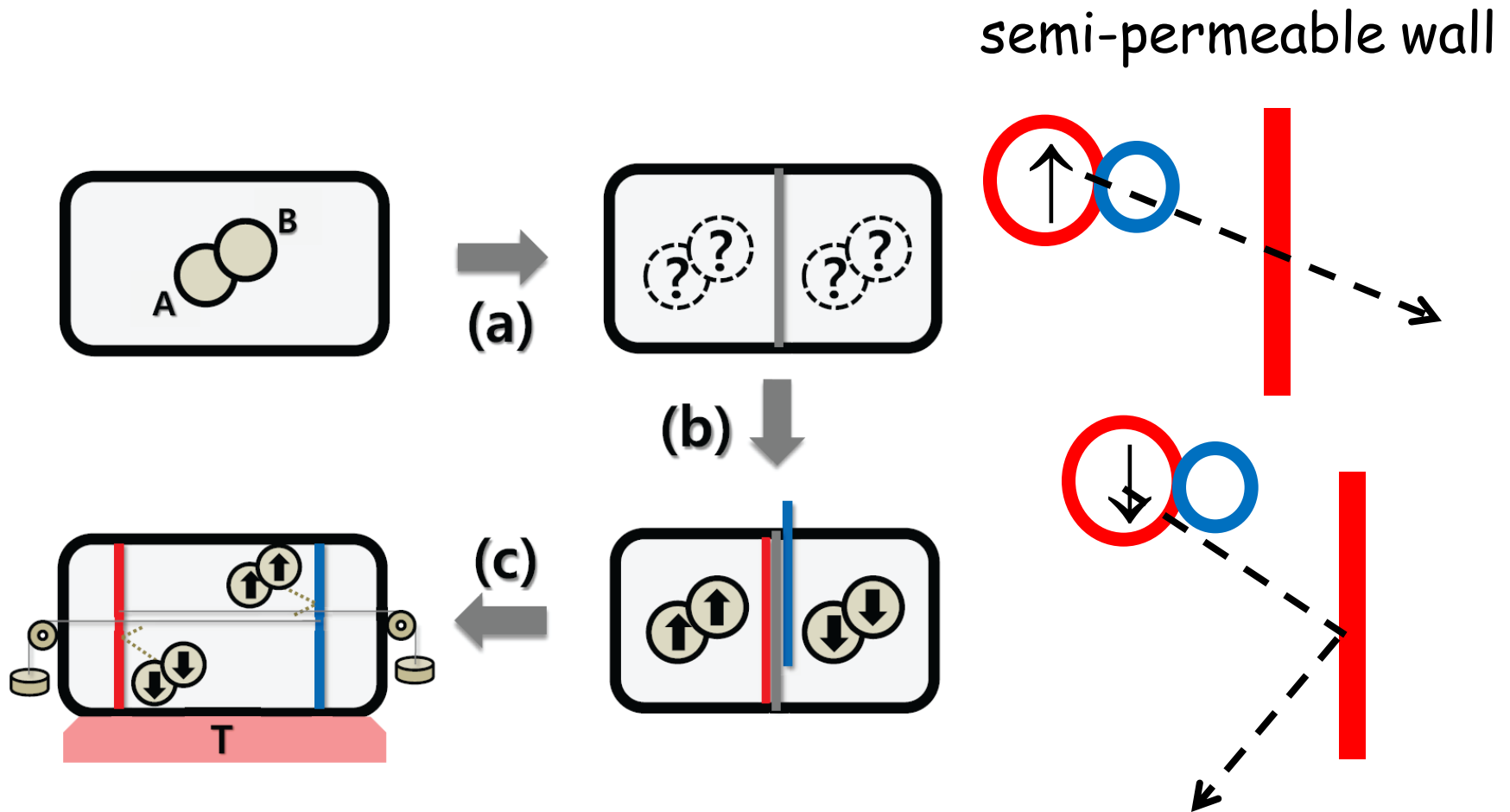
quantum discord  $\mathcal{D}(B | A) = \min \left[ I(A : B) - \tilde{J}_{\{\Pi_A^i\}}(B : A) \right]$

# Final formula

$$W \leq -\Delta F_S + kT(\Delta S_A + \Delta S_B) - kT\Delta J + kT\delta(B^{(i)}|A^{(i)})$$




# Szilard engine containing a heteronuclear diatomic molecule



$$\rho^{(1)} = |\Psi^+\rangle_{AB} \langle \Psi^+| \otimes \frac{1}{2} (|L\rangle_S \langle L| + |R\rangle_S \langle R|) \otimes \rho_R^{\text{can}} \quad |\Psi^+\rangle_{AB} = \frac{1}{\sqrt{2}} (|\uparrow_A \uparrow_B\rangle + |\downarrow_A \downarrow_B\rangle)$$

$$U^{(2)} = \frac{1}{2} (|\uparrow\uparrow\rangle \langle \Psi^+| \otimes |L\rangle \langle L| + |\downarrow\downarrow\rangle \langle \Psi^+| \otimes |R\rangle \langle R|)$$


 $\Pi_A^k \in \{|\uparrow\rangle_A \langle \uparrow|, |\downarrow\rangle_A \langle \downarrow|\}$

$$\rho^{(12)} = \frac{1}{2} (|\uparrow\uparrow\rangle \langle \uparrow\uparrow| \otimes |L\rangle_S \langle L| + |\downarrow\downarrow\rangle \langle \downarrow\downarrow| \otimes |R\rangle_S \langle R|) \otimes \rho_R^{\text{can}}$$

$$\rho^{(f)} = \frac{1}{2} (|\uparrow\uparrow\rangle \langle \uparrow\uparrow| + |\downarrow\downarrow\rangle \langle \downarrow\downarrow|) \otimes \frac{1}{2} (|L\rangle_S \langle L| + |R\rangle_S \langle R|) \otimes \rho_R^{\text{can}}$$

$$W \leq -\Delta F_S + kT(\Delta S_A + \Delta S_B) - kT\Delta J + kT\delta(B^{(i)} | A^{(i)})$$

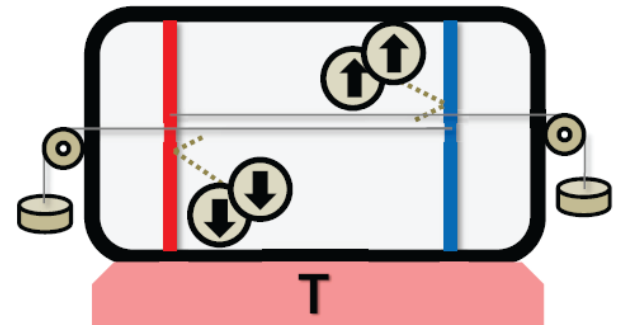
$$\Delta F_S = 0 \quad \Delta S_A = \Delta S_B = 0 \quad \Delta J = 0$$

$$I(A^{(i)} : B^{(i)}) \equiv S(\rho_A^{(i)}) + S(\rho_B^{(i)}) - S(\rho_{AB}^{(i)})$$

$$= \ln 2 + \ln 2 - 0 = 2 \ln 2$$

$$\delta(B^{(i)} | A^{(i)}) = \min [I(A : B) - \tilde{J}_{\{\Pi_A^i\}}(B : A)]$$

$$= 2 \ln 2 - \ln 2 = \ln 2$$



$$W = \frac{1}{2} kT \ln 2 + \frac{1}{2} kT \ln 2 = kT \ln 2$$

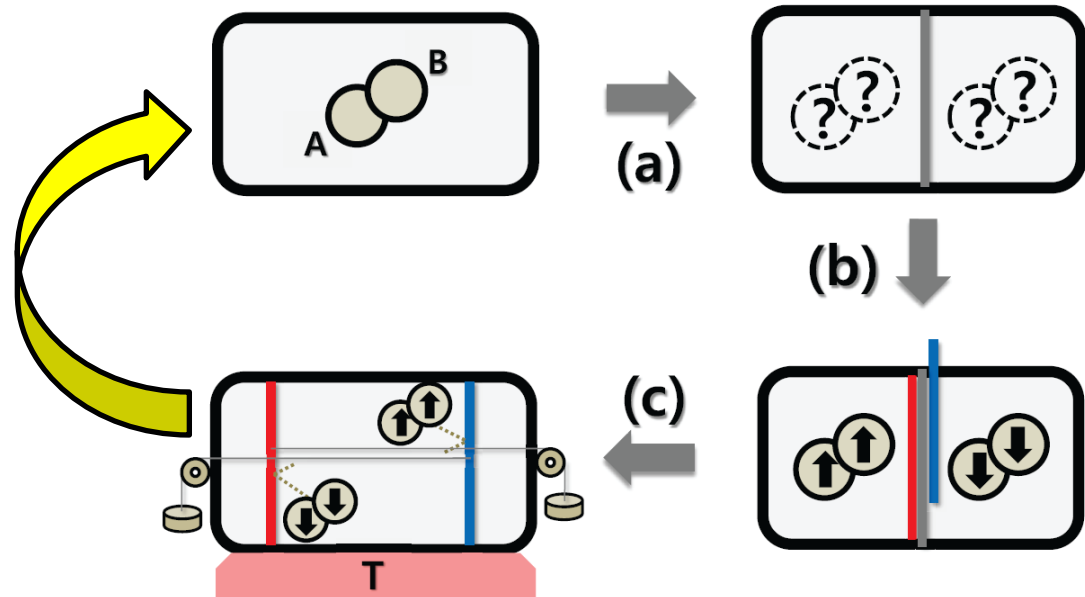
# Thermodynamic 2nd law

$$\rho^{(f)} = \frac{1}{2} \left( |\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow| \right) \otimes \frac{1}{2} \left( |L\rangle_S\langle L| + |R\rangle_S\langle R| \right) \otimes \rho_R^{\text{can}}$$

$$\rho^{(1)} = |\Psi^+\rangle_{AB} \langle\Psi^+| \otimes \frac{1}{2} \left( |L\rangle_S\langle L| + |R\rangle_S\langle R| \right) \otimes \rho_R^{\text{can}}$$

$$S[\rho^{(f)}] - S[\rho^{(1)}] = \ln 2$$

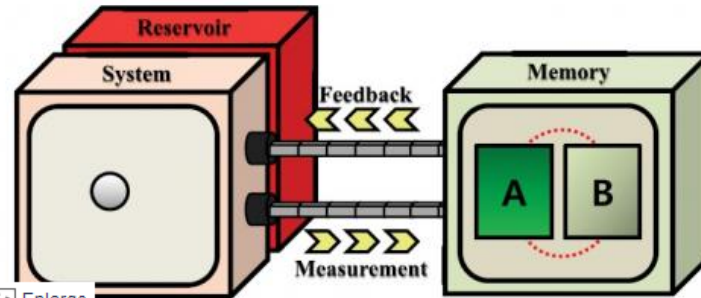
To prepare the initial state of memory, we need to pay  $kT \ln 2$ .





# Maxwell's demon can use quantum information

Dec 18, 2013 by Lisa Zyga feature



Enlarge

In the quantum information heat engine, the system is attached to the reservoir, and is measured and controlled by the memory consisting of a diatomic molecule with two entangled states. Credit: Park, et al. ©2013 American Physical Society

(Phys.org) —In theory, Maxwell's demon can decrease the entropy of a system by opening and closing a door at appropriate times to separate hot and cold gas molecules. But as physicist Leó Szilárd pointed out in 1929, entropy does not decrease in such a situation because the demon's measurement process requires information, which is a form of entropy. Szilárd's so-called information heat engine, now called the Szilárd engine (SZE), demonstrates how work can be generated by using information.



Q-info demon

Park, K.-H. Kim, Sagawa & SWK, PRL (2013)

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# Summary

A photograph of a night festival or fireworks display. In the foreground, a person's arm is visible on the left, pointing towards the center. In the middle ground, a person is holding a bright sparkler. To the right, another person is holding a large firework that is exploding, creating a large plume of orange and yellow light. The background is dark with several bright spots of light, possibly other fireworks or streetlights. The overall scene is festive and brightly lit by the artificial light of the fireworks.

- We have studied quantum dynamical SZE.
- We have found optimal condition of quantum SZE with irreversibility
- We have devised Maxwell demon utilizing quantum information (q-discord)



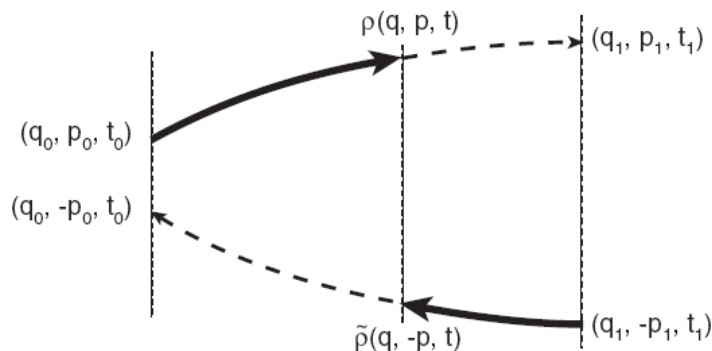
# Non-equilibrium thermodynamics

- Jarzynski equality (1997)

$$\left\langle e^{-\beta W} \right\rangle_{\text{non-equilibrium}} = e^{-\beta \Delta F}$$

-The dissipative work for non-equilibrium process

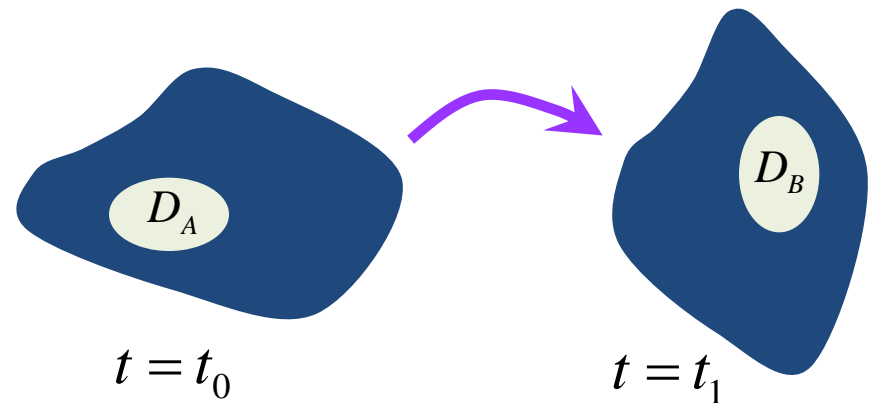
$$\langle W \rangle_{\text{diss}} = \langle W \rangle - \Delta F = kT \left\langle \ln \frac{\rho}{\tilde{\rho}} \right\rangle_{\rho}$$



Kawai, Parrando & Van den Broeck,

-The dissipative work for non-equilibrium process with filtering or feedback control

$$kT \left\langle \ln \frac{\rho}{\tilde{\rho}} \right\rangle_{\rho} + kT \ln \frac{P_{D_A}}{P_{D_B}} = \langle W \rangle - \Delta F$$



Parrando, Van den Broeck & Kawai,

New J. Phys (2009)

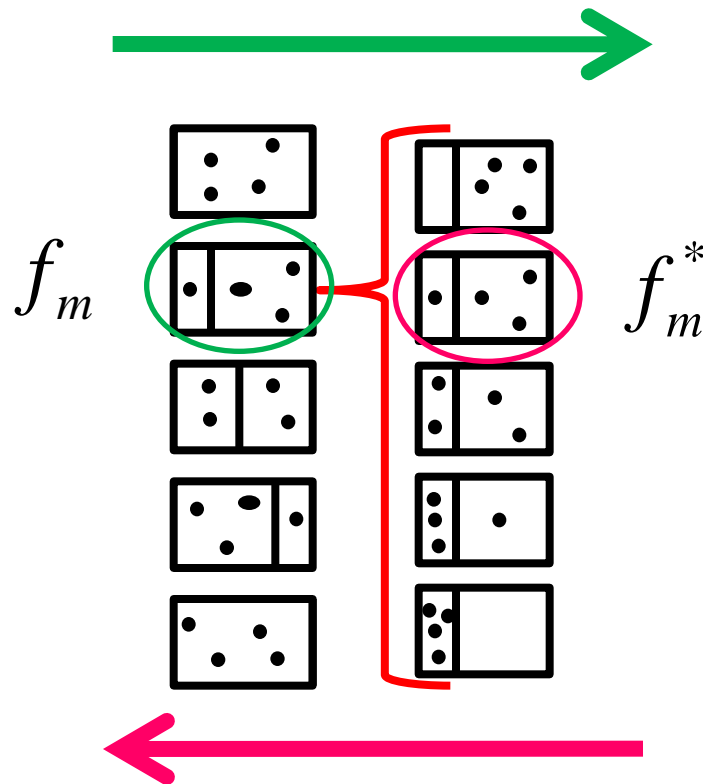
# Physical meaning of $-\sum f \ln(f/f^*)$

$$\cancel{kT \left\langle \ln \frac{\rho}{\tilde{\rho}} \right\rangle_{\rho}} + kT \ln \frac{p_{D_A}}{p_{D_B}} = \langle W \rangle - \cancel{p_{D_A} F}$$

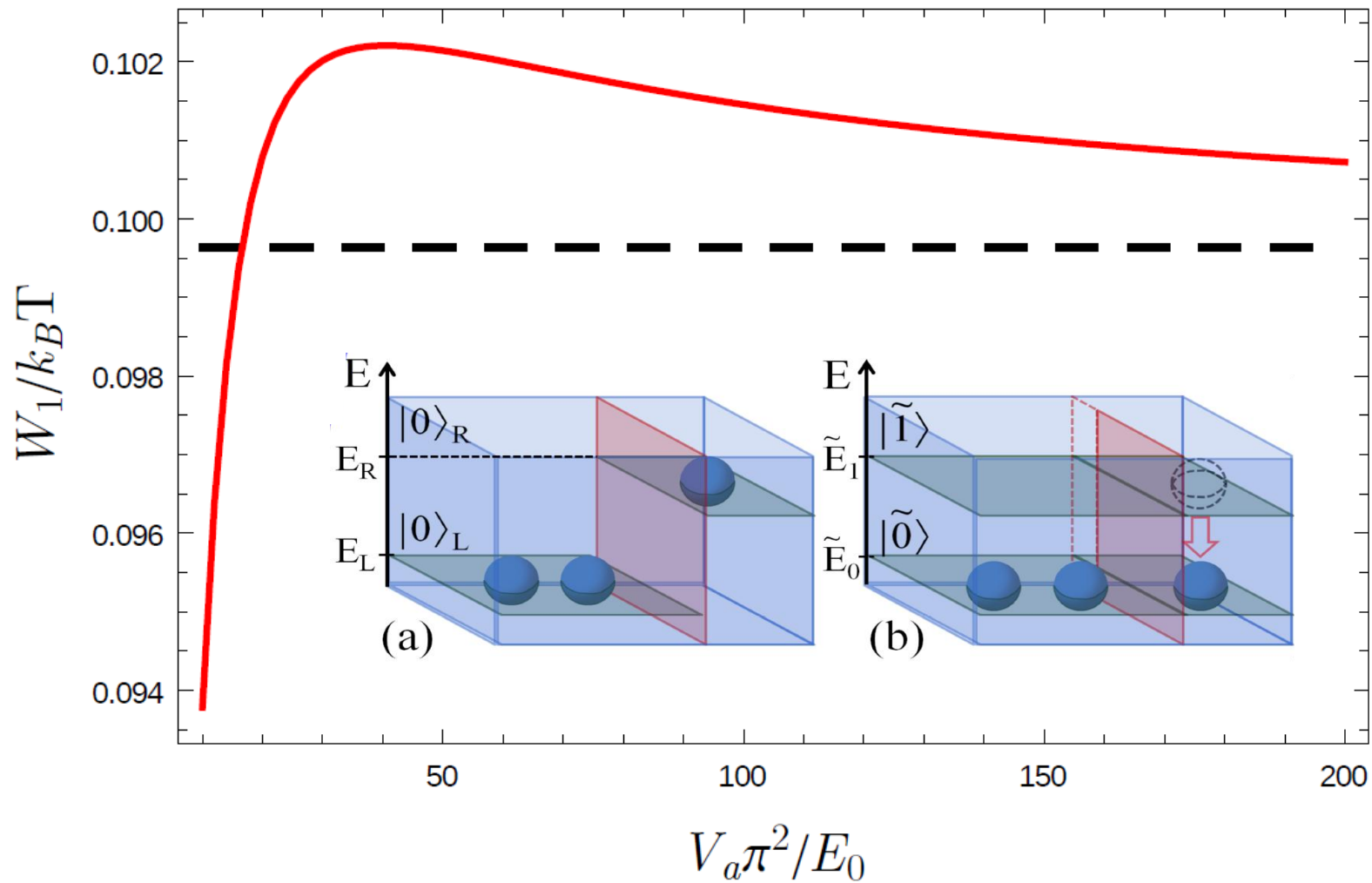
quasi-static process
cyclic engine

forward filtering  $p_{D_A} = f_m$   
 backward filtering  $p_{D_B} = f_m^*$

$$\begin{aligned}
 \langle W \rangle_{tot} &= \sum_m f_m \langle W \rangle_m \\
 &= kT \sum_m f_m \ln \left( \frac{f_m}{f_m^*} \right)
 \end{aligned}$$



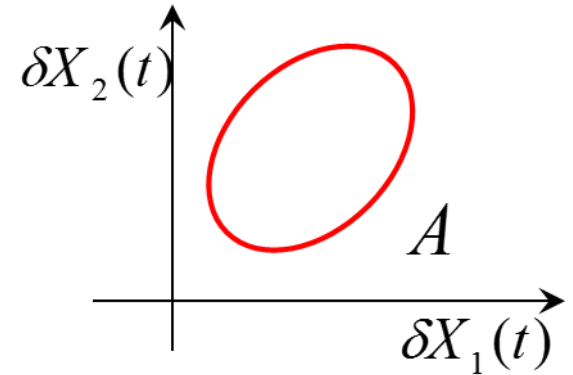
# Remark I



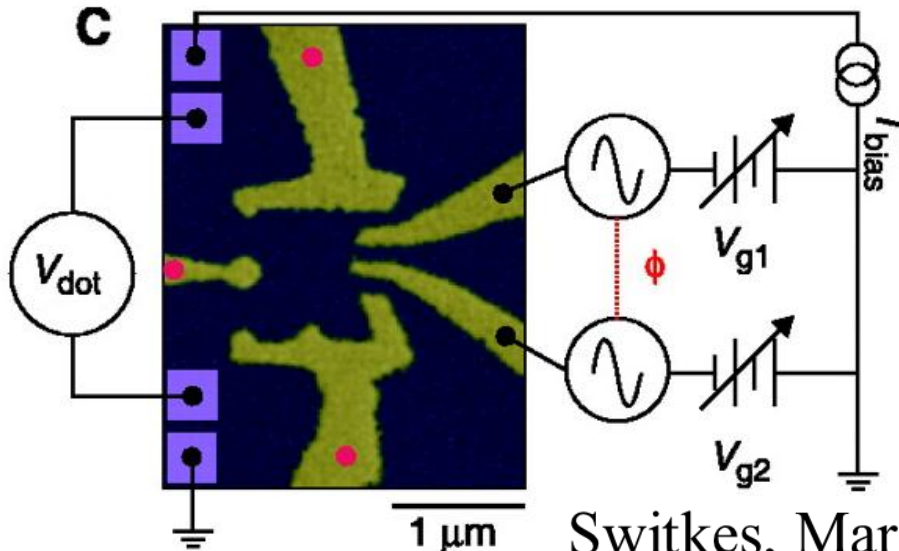
# Adiabatic Q-pump

$$Q(m) = \frac{e}{\pi} \int_A dX_1 dX_2 \sum_{\beta, \alpha \in m} \text{Im} \frac{\partial S_{\alpha\beta}}{\partial X_1} \frac{\partial S_{\alpha\beta}^*}{\partial X_2}$$

$$\delta X_1(t) = \delta X_1 \sin \omega t, \delta X_2(t) = \delta X_2 \sin(\omega t + \phi)$$



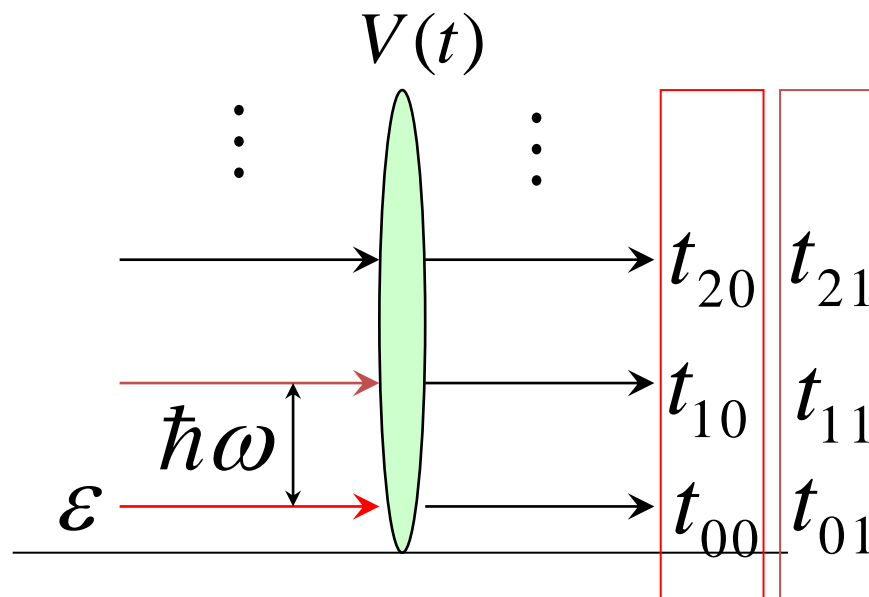
Brouwer (1998)



Switkes, Marcus, Campman, and Gossard (1999)

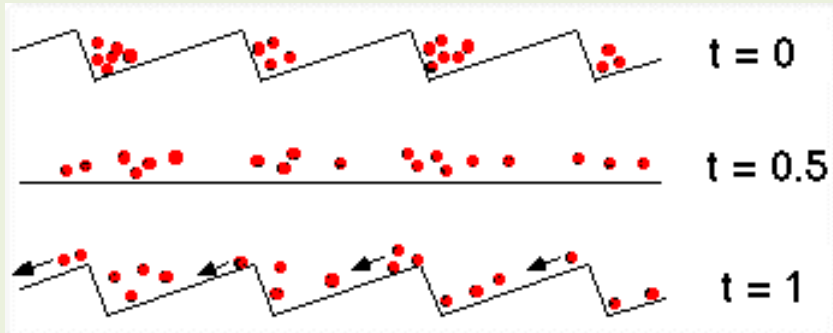


$$S = \begin{pmatrix} r_{00} & r_{01} & \cdots & t_{00}' & t_{01}' & \cdots \\ r_{10} & r_{11} & \cdots & t_{10}' & t_{11}' & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\ t_{00} & t_{01} & \cdots & r_{00}' & r_{01}' & \cdots \\ t_{10} & t_{11} & \cdots & r_{10}' & r_{11}' & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \end{pmatrix}$$

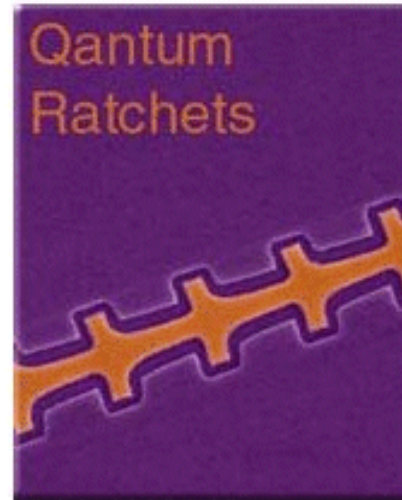


$$I = \frac{2e}{h} \int dE dE' [t_{\rightarrow}(E', E) f_L(E) - t_{\leftarrow}(E, E') f_R(E')]$$

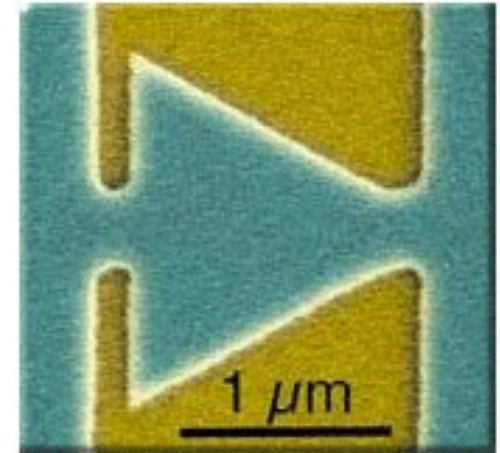
# Classical/Quantum ratchet



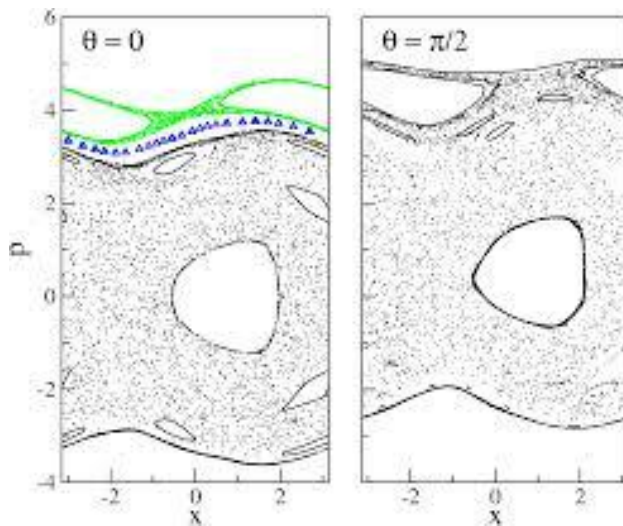
Classical ratchet



SEM image of a tunneling ratchet (highlighted in orange)



Electron microscopic image of a quantum dot ratchet



<http://www.uoregon.edu/~linke/>