Quantum heat engine using energy quantization in potential barrier

Sibasish Ghosh

Optics and Quantum Information Group
The Institute of Mathematical Sciences
C.I.T. Campus, Taramani
Chennai–600113.

[In collaboration with George Thomas (IMSc Chennai) and Debmalya Das (HRI Allahabad)]

ISNFQC 2018

31 January, 2018

Motivation 1

Quantum thermodynamics

To extend thermodynamics in quantum regime.

- Superposition and entanglement
- Quantum processes such as quantum adiabatic process, quantum measurement
- A few particle system in a thermal environment
- Distinguishable vs. indistinguishable particles

Models

Quantum thermodynamic machines

Motivation 2

- Maxwell's Demon: Thought experiment introduced by Maxwell in 1872 to show an apparent violation of Second law of thermodynamics.
- Szilard engine: Introduced by Szilard in 1929 to illustrate Maxwell's Demon using single molecule gas.
- Subtle connection with information and thermodynamics: The apparent violation of Second law was solved if the amount of amount of heat dissipated while erasing the memory (Landauer's erasure principle) is considered. [1]
- Experimental realizations of Maxwell's Demon and quantum heat engines and confirmation of erasure principle. [2]
- Quantum Szilard engine: The insertion and the removal of the barrier also involves work. [3]

---

[1] R. Landauer, IBM J. Res. Dev. **5**, 183 (1961).
C. H. Bennett, Int. J. Theor. Phys. **21**, 905 (1982).

[2] J.V. Koski et al, Phys. Rev. Lett. 115, 260602 (2015).
A. Bérut et al, Nature **483**, 187 (2012)
D.Gelbwaser-Klimovskya et al, arXiv:1705.11180 [quant-ph] (2017)

[3] S.W. Kim et al, **106**, 070401 (2011).

Our focus

- To model a quantum heat engine having exclusively quantum features. [4]
- To show that the lack of information can also be a useful resource.
- To study the performance of distinguishable particles and indistinguishable (Bosons and Fermions) in a quantum heat engine.

[4] Previous studies on quantum Otto cycle enabled by energy quantization; D.Gelbwaser-Klimovskya et al, arXiv:1705.11180 [quant-ph] (2017).

Outline

- Maxwell's demon
- Quantum Szilard engine
- Lack of information and work
- Quantum Stirling engine
- Limiting cases
- Engine with indistinguishable particles
- Conclusion and open questions

Maxwell's demon

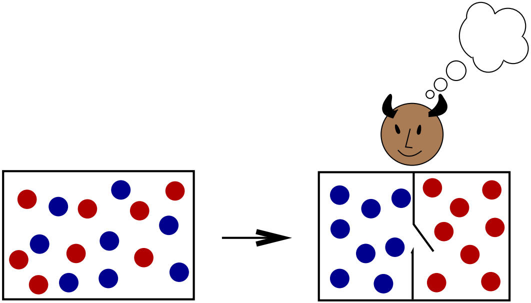


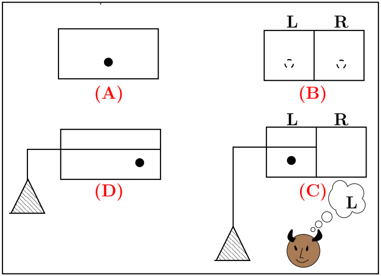
Figure: Maxwell's demon allows the gas molecules with higher velocities to the right and molecules with lower velocities to the left. This creates a temperature gradient between left and right chambers. Further, this temperature gradient can be used to extract work

5

[5] H. Leff and A. F. Rex, Maxwells Demon 2: Entropy, Classical and Quantum Information, Computing (Institute of Physics, Bristol, 2003).

Quantum Szilard engine

Quantum Szilard engine



- (A) A particle in a box
- (B) Insertion of the barrier
- (C) Measurement: to know whether the particle in 'L' or 'R'.
- (D) Isothermal expansion: this leads to the lifting up of the load. [6]
- *Classical case:* Work required to insert the barrier is zero.
- *Quantum case:* Work required to insert the barrier is non-zero.[7]

[6] L. Szilard, Zeitschrift fr Physik 53, 840 (1929).

[7] S.W. Kim et al, Phys. Rev. Lett. **106**, 070401 (2011).

Quantum Szilard engine with many particles

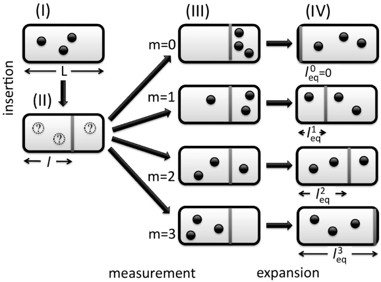


Figure: Schematic diagram of the quantum SZE containing three molecules. (I) Three molecules are prepared in a closed box with size L. (II) A wall, depicted by a vertical gray bar, is isothermally inserted at location l. The process $(I) \to (II)$ is called insertion. (III) The information on the number of molecules, m, on the left is acquired by the measurement. The process $(II) \to (III)$ is called measurement. (IV) The wall moves and undergoes an isothermal expansion until it reaches its equilibrium location denoted by l_{eq}^{m} eq . The process $(III) \to (IV)$ is called expansion. Finally the wall is isothermally removed to complete the cycle. The process $(IV) \to (I)$ is called removal.

S.W. Kim et al, Phys. Rev. Lett. **106**, 070401 (2011).

Particle in box

Energy eigenvalues and eigenfunctions

$$E_n = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

$$\psi_n = \sqrt{\frac{1}{a}}\sin\left(\frac{n\pi}{2a}x\right)$$

where $n = 1, 2, 3, \cdots$.

Particle in a box with delta potential in the center

$$\begin{aligned} & = & \infty & \quad x < -a \\ V(x) & = & \alpha\delta(x) & \quad -a < x < a \\ & = & \infty & \quad x > a \end{aligned}$$

ψ_2, ψ_4, ... (E_2, E_4, ...) remains unchanged.
ψ_1, ψ_3, ... (E_1, E_3, ...) are modified.
For $\alpha \to \infty$, $E_1 = E_2$, $E_3 = E_4$, ...

- Consider a particle in a box of length $2a$ and in equilibrium with a bath of temperature T. Let the canonical partition function be $Z(2a)$.
- Now, consider a process in which isothermally inserting barrier in the middle of the box. The partition function at the end of the process is $Z_{\rm fin} = 2Z(a)$ where $Z(a)$ is partition function for particle trapped in box of length a.
- The factor 2 appears because of the degeneracy or in other words, due to the ignorance about the particle being in the left or right side of the box.
- Therefore, the work done by the engine is the difference in free energy, $W_{\rm insertion} = k_B T[\ln 2 + \ln Z(a) - \ln Z(2a))]$. This work is lesser than the work needed to compress the box from $2a$ to a.
- Work needed for isothermal compression, $W_{\rm comp} = k_B T[\ln Z(a) - \ln Z(2a))]$
- As compared to isothermal compression, during the isothermal insertion, there is a lack of information i.e. whether the particle is on the left or right side of the box, which leads to a difference of $k_B T \ln 2$ in the work. The implication of this term will be seen later.

Quantum Stirling engine

Classical Stirling cycle

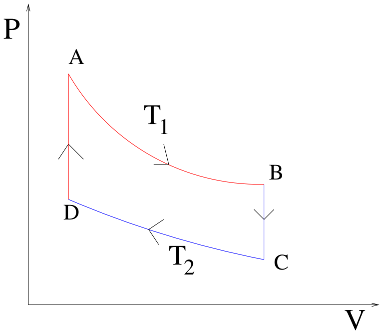
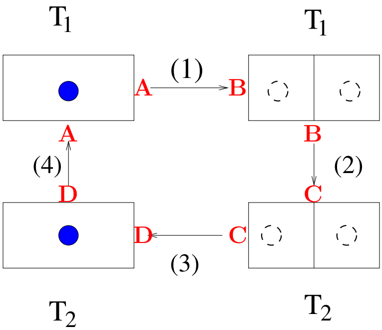


Figure: Stirling cycle: AB and CD are isothermal processes. BC and DA are isochoric (constant volume) processes. System is in contact with hot bath during DA and AB. The system is in contact with cold bath during BC and CD. In classical Stirling cycle, the working medium is ideal gas and it can work at Carnot efficiency.

Quantum Stirling Cycle



- Stage 1: (A-B) Isothermal insertion of the barrier.
- Stage 2: (B-C) Isochoric process, temperature of the system changes from T_1 to T_2 at constant volume.
- Stage 3: (C-D) Isothermal removal of the barrier.
- Stage 4: (D-A) Isochoric process, temperature of the system changes from T_2 to T_1 at constant volume.

$$E_n = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}, \quad Z_A = \sum_n e^{-\frac{E_n}{k_B T_1}}$$

$$E_{2n} = \frac{(2n)^2\pi^2\hbar^2}{2m(2a)^2}, \quad Z_B = \sum_n 2e^{-\frac{E_{2n}}{k_B T_1}}$$

The heat exchanged in the isothermal process of introducing the wall in Stage 1 is thus,

$$Q_h = U_B - U_A + k_B T_1 \log Z_B - k_B T_1 \log Z_A$$

$$Q_h = \sum_n \left(\frac{\frac{(2n)^2\pi^2\hbar^2}{2m(2a)^2} 2e^{-\frac{(2n)^2\pi^2\hbar^2}{2m(2a)^2 k_B T_1}}}{Z_B} - \frac{\frac{n^2\pi^2\hbar^2}{2m(2a)^2} e^{-\frac{n^2\pi^2\hbar^2}{2m(2a)^2 k_B T_1}}}{Z_A} \right) - k_B T_1 \ln Z_A + k_B T_1 \ln Z_B \qquad (1)$$

Heat (continued)

Similarly, during the isochoric process (Stage 2)

$$Q'_c = U_C - U_B$$

Similarly, the heat exchanged in Stage 3 and Stage 4.

$$Q_c = U_D - U_C + k_B T_2 \log Z_D - k_B T_2 \log Z_C$$

and

$$Q'_h = U_A - U_D$$

Work and efficiency

$$W = k_B T_1 (\log \frac{Z_B}{Z_A}) - k_B T_2 (\log \frac{Z_C}{Z_D})$$

$$\eta = 1 + \frac{Q_c + Q'_c}{Q_h + Q'_h}$$

Plotting work

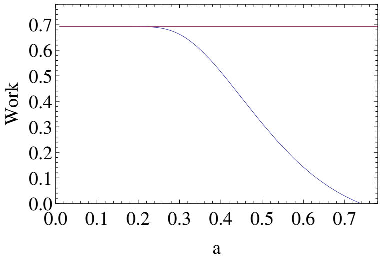


Figure: Plot of total work vs the a. The horizontal line represents the limiting case $(T_1 - T_2)\ln 2$. Here, we have taken $T_1 = 2$ and $T_2 = 1$. We set $k_B = 1$.

Plotting efficiency

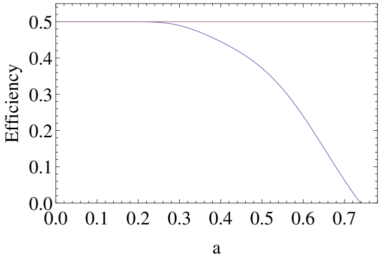


Figure: Plot for Efficiency vs a. The horizontal line represents the Carnot efficiency $(1 - \frac{T_2}{T_1})$ obtained from the limiting case. Here, we have taken $T_1 = 2,\ T_2 = 1$ and $k_B = 1$.

Limiting cases

Classical limit

The energy difference between the two adjacent levels (nth and (n+1)th) are $(2n+1)\pi^2\hbar^2/2m(2a)^2$. During the insertion of the barrier, the odd energy levels approaches the next even numbered level. When the barrier is fully inserted, each energy level will be doubly degenerate. Therefore the gap between the adjacent energy levels is responsible for the work. When $a \to \infty$, the energy gap goes to zero and there will be a continuum of energy levels. Therefore the work required to insert or remove the barrier goes to zero.

Low temperature limit

Let us consider a box with length $2a$ such that $3\pi^2\hbar^2/2m(2a)^2 >> k_B T_1$. In this case, the occupational probability in the ground state is close to unity and entropy approaches zero. When the partition is inserted, the ground state of the double well becomes doubly degenerate with occupational probability $1/2$ for each states and hence the entropy becomes $\ln 2$. Therefore the total heat absorbed from the hot bath becomes $T_1 \ln 2$. Similarly when the wall is removed, the heat exchanged is $-T_2 \ln 2$. Therefore the work done and the efficiency in this case becomes

$$W = k_B(T_1 - T_2)\ln 2, \quad \eta = 1 - \frac{T_2}{T_1}$$

As seen earlier, $k_B T \ln 2$ appears due to the lack of information about the position of the particle during insertion and removal of the barrier.

Engine with indistinguishable particles

Indistinguishable particles

$$\Psi_{B/F} = \frac{1}{\sqrt{2}}[\psi_m(x_1)\psi_n(x_2) \pm \psi_n(x_1)\psi_m(x_2)]$$

Ground state of Bosons : $n = 1$ and $m = 1$.
Ground state of Fermions : $n = 1$ and $m = 2$.

Statistics of the particles

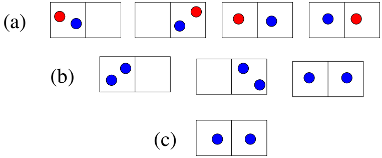


Figure: Particle statistics after inserting the barrier: (a) Distinguishable particles, (b) Bosons and (c) Fermions.

Comparison with indistinguishable particles

No. of ways of arranging n particles in g boxes (with (g-1) barriers):
Distinguishable particles: g^n
Bosons : $(n+g-1)!/n!(g-1)!$
Fermions : $g!/n!(g-n)!$

Table: Comparison of work for the case of 2 particles.

Particles	Bar.No.	.	Work
Distinguishable	1		$2k_B(T_1 - T_2)\ln 2$
Fermions	1		0
Bosons	1		$k_B(T_1 - T_2)\ln 3$
Distinguishable	2		$2k_B(T_1 - T_2)\ln 3$
Fermions	2		$k_B(T_1 - T_2)\ln 3$
Bosons	2		$k_B(T_1 - T_2)\ln 6$

Comparison with indistinguishable particles

Table: Comparison for the case of 3 particles.

Particles	Bar.No.	.	Work
Distinguishable	1		$3k_B(T_1 - T_2)\ln 2$
Fermions	1		$k_B(T_1 - T_2)\ln 2$
Bosons	1		$2k_B(T_1 - T_2)\ln 2$
Distinguishable	2		$3k_B(T_1 - T_2)\ln 3$
Fermions	2		0
Bosons	2		$k_B(T_1 - T_2)\ln 10$

Conclusion and future directions

Conclusion

- We have seen quantum model of Stirling engine which uses exclusively quantum features (quantization of energy levels).
- Classical limit and low temperature limits are obtained.
- Lack of information of the position of the particle can be converted to work.
- Work obtained from distinguishable particles, Fermions and bosons are different.

Future directions:

- To study finite time model of the heat engine.
- Effect of having interaction/correlations among the particles
- Efficiency at maximum power.
- Physical realization of the heat engine.

Thanks