Asian Journal of Physics
Vol. 26, No 1 (2017) 21-26
Available on: www.asianjournalofphysics.in

Quantum engine cycles and shape of the trap

Dario Poletti
Singapore University of Technology and Design, 8 Somapah Road, 487372 Singapore and
Maju Lab, CNRS-UNS-NUS-NTU International Joint Research Unit, UMI 3654, Singapore

We review some critical aspects related to the shape of traps confining a gaseous working fluid and its consequences on the performance of quantum engines cycles. We show that when the gas trapping potential has a particular shape, the state of the gas can remain thermal after a quantum adiabatic transformation. We then discuss the comparison of engine cycles for gases confined in traps of different geometrical forms. We conclude by analyzing the interplay between the quantum statistics of the particles constituting the working fluid and the shape of the trap.

Keywords: Quantum thermodynamics, Ion traps

1 Introduction

Classical and macroscopic heat engines are extremely important in our daily lives. They allow the conversion of a form of energy, known as heat, to another form of energy, known as work, through transformations in a working fluid. Heat carries entropy while work does not. The laws of thermodynamics teach us the limits within which such conversion is possible [1]. In particular not all the heat transferred can be converted into work.

It is important to uncover the details of heat to energy conversion also at the nanoscale, in regimes in which the laws of quantum mechanics need to be applied. Large energy savings would result if it was possible to efficiently convert heat into work at the nanoscale. The quest for a deeper understanding of the basic fundamental limits of thermodynamics and good design principles for future quantum thermodynamic systems has started.

One of the earliest works studied the functioning of a maser as a heat engine [2]. This interest was revived more recently, and the community is now focused on three general types of engines: self-contained, continuously driven and stroke engines. For the latter type of engines, the cycle is divided in a distinct and discrete sequence of processes (strokes). Typical examples studied in the literature are the Carnot cycle (composed of two adiabatic and two isothermal processes) and the Otto cycle (composed of two adiabatic and two isochoric processes). In these two cycles, for instance, the heat baths are coupled to the engine only for certain intervals. In continuously driven engines the baths are always in contact with a working fluid which is periodically driven by some external potential. The last important class of engines is the self-contained, autonomous, engines, in which the engine and the load are considered together, and no external driving mimics the effects of the load on the engine [2-7]. Reviews which discuss the above topics are [8-18].

In the following we concentrate on a particular type of stroke cycle which is the Otto cycle. We will discuss the important role played by the shape of the trap during a quantum adiabatic process, in the performance of an engine, and its interplay with the statistics of the working fluid.

Corresponding author :
e-mail: dariopoletti@gmail.com.(Dario Poletti)

2 Quantum adiabatic processes and Gibbs states

An adiabatic process is a reversible process with no heat exchange, only work transfers. It is modelled by an (infinitely slow) Hamiltonian evolution for which the entropy of the system does not increase. This can be readily shown by considering Von Neumann entropy S of a density matrix $\hat{\rho}$,

$$S = \mathrm{tr}\,[\hat{\rho}\ln(\hat{\rho})] \tag{1}$$

whose time derivative is given by

$$\begin{aligned}\frac{dS}{dt} &= \mathrm{tr}\left[\frac{d\hat{\rho}}{dt}\ln(\hat{\rho})\right] + \mathrm{tr}\left[\frac{d\hat{\rho}}{dt}\right] \\ &= \mathrm{tr}\left[-i[\hat{H},\hat{\rho}]\ln(\hat{\rho})\right] \\ &= \mathrm{tr}\left[-i[\hat{\rho},\ln(\hat{\rho})]\hat{H}\right] \\ &= 0\end{aligned}$$

where $\hat{H}$ is the Hamiltonian operator. For the derivation we have used the trace-preserving property of the Hamiltonian evolution, and the invariance of cyclic permutations in the trace (this is indeed true also for finite time processes). If we now consider a quantum system with discrete energy levels undergoing an infinitely slow process, then the entropy is conserved, and the occupation of each energy level is kept constant.

It is thus clear that, in general, a quantum adiabatic transformation does not keep the density matrix in a thermal-like form. For a Gibbs state to remain in such a form (although at a different temperature) if the potential fulfills a scale-invariant property. To be more general, we now consider a many body system of N particles. A scaling potential V is such that

$$V(x_i) = \frac{1}{\lambda^2} f\left(\frac{x_i}{\lambda}\right) \tag{2}$$

for a particle at position x_i. λ is a scaling parameter. This is due to the fact that

$$\begin{aligned}\hat{H} &= \sum_i \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2} + \frac{1}{\lambda^2} f\left(\frac{x_i}{\lambda}\right)\right] \\ &= \frac{1}{\lambda^2}\sum_i \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial X_i^2} + f(X_i)\right] \\ &= \frac{1}{\lambda^2}\hat{h}\end{aligned} \tag{3}$$

where $X_i = x_i/\lambda$ is a dimensionless variable. It follows that, for a quantum adiabatic transformation in which the parameter λ is changed to λ', a thermal state, which was initially at inverse temperature β, remains thermal, however at a different temperature $\beta' = (\lambda'/\lambda)^2\beta$. This can be shown by the following computation

$$\exp\left(-\beta\hat{H}\right) = \exp\left(-\beta\frac{1}{\lambda^2}\hat{h}\right) = \exp\left(-\beta\frac{\lambda'^2}{\lambda^2}\frac{1}{\lambda'^2}\hat{h}\right) = \exp\left(-\beta'\frac{1}{\lambda'^2}\hat{h}\right) \tag{4}$$

In scale-invariant potentials it is also easy to compute the work exchanged during a quantum adiabatic process. For work, W, we use the two-times measurement definition [19-21]. Work being a fluctuating quantity, its probability distribution $P(W)$ is given, for a process between time $t = 0$ to $t = \tau$, by

$$P(W) = \sum_{n,m} \delta\,(W - (E'_m - E_n))\,P_{0,\tau}^{n,m}\,p_n, \tag{5}$$

where E_n is the n-th eigenvalue of the Hamiltonian at time $t = 0$, while P_n is the probability of it being occupied, E'_m is the m-th eigenvalue of the Hamiltonian at time $t = 0$, and $P_{0,\tau}^{n,m}$ is the transfer probability between the states n and m. In a quantum adiabatic process $P_{0,\tau}^{n,m} = \delta_{n,m}$ and $E'_m = (\lambda/\lambda')^2\ E_m$, because of the use of a scale-invariant potential, the work can hence be easily written as

$$\langle W^{ad}\rangle_{0,\tau} = \left[\left(\frac{\lambda}{\lambda'}\right) - 1\right]\sum_n E_n P_n$$
$$= \left[\left(\frac{\lambda}{\lambda'}\right) - 1\right]\langle E\rangle_0 \tag{6}$$

where $\langle E\rangle_0$ is the average energy of the state at time $t = 0$. The variance of the work output can also be computed from

$$\sigma_{\mathrm{W}}^2 = \sum_n \left[\left(\frac{\lambda}{\lambda'}\right) - 1\right]^2 E_n^2\, P_n\, \langle W^{ad}\rangle_{0,\tau}^2 = \left[\left(\frac{\lambda}{\lambda'}\right) - 1\right]^2 \sigma_{E_0}^2 \tag{7}$$

where

$$\sigma_{E_0}^2 = \sum_n E_n^2\, P_n\, \langle E\rangle_0^2 \tag{8}$$

is the variance of the energy at $t = 0$.

Another significant advantage of using scale-invariant potentials is that it is possible to derive explicitly a counterdiabatic driving for them [22] (although the energetic cost of applying a driving field should also be carefully considered [23]). The effect of a non-thermal-like distribution in a Carnot cycle has been studied in [24].

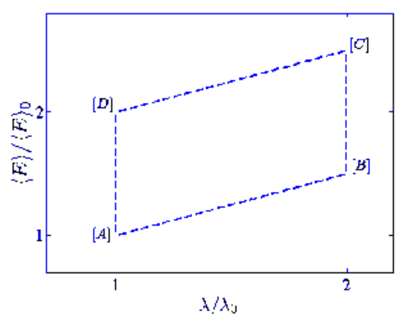

Fig 1. Schematics of a quantum Otto Cycle. The four strokes are: from vertex [A] to [B] adiabatic contraction, from [B] to [C] isoparametric heating, [C] to [D] adiabatic expansion and from [D] to [A] isoparametric cooling. The x axis represents the change of the scaling parameter λ from its initial value λ_0, while the y axis represents the change in the average energy $\langle E\rangle = (\hat{H}\hat{\rho})$ compared to $\langle E\rangle_0$ which is the value at [A].

3 Otto cycles with scale-invariant potentials

The fact that a state remains thermal during a quantum adiabatic process allows a clear study of its thermodynamic properties. In [25] the authors studied the role of the shape of the trap for an Otto cycle. At this point it is important to make some remarks. First of all, for the isochoric process of a classical Otto cycle, the volume is constant as the trap is kept at a xed shape and the temperature is changed. Since the volume does not change, no work is done or received. However, for a quantum gas, if a trap is kept constant and the temperature is increased, the volume of the gas, measured (in one dimension) as $v = \mathrm{tr}(x^2\hat{\rho})$, does not remain constant. However, as in the classical case, since the traping potential has not changed, no work has been done nor received by the gas. We will thus preferably use the expression of isoparametric instead of isochoric. The second remark is that the comparison of the performance of Otto cycles in different traps, for example a trap characterised by the potential $V_1 = 1/\lambda^2 f_1(x/\lambda)$ and a second one with a potential $V_2 = 1/\lambda^2 f_2(x/\lambda)$, requires a more detailed specification of the set-ups. In fact it is necessary to assign at least two parameters to fully specify a thermal density operator, β and λ, which can be identified either by a choice of the temperature and the volume, or the temperature and the energy. The full cycle is determined by two vertices, for example vertices [A] and [C] of Fig.1 and hence by 4 parameters, e.g. the volume and temperature at point [A] and energy and entropy at point [C]. Interestingly, it is indeed possible to set two cycles such that the energy at the 4 vertices is the same in each of them. This implies that all the energy exchanges are the same between the two cycles, and hence the work exchanged and the efficiency are also identical between them. It would thus seem that there may not be any relevance to study different traps. However, energy exchanges are simply average values, and what is also important is the distribution of the energy exchanges, especially for small systems. The net work probability distribution, for two cycles which have the same average energy exchanges, can vary significantly depending on the shape of the trap [25].

To summarize this section, for a fair comparison between Otto engine cycles done with two different scale-invariant traps, it is important to specify in a detailed enough manner, the conditions of comparison (temperatures, volumes, energies at the vertices). Moreover, even if the average energy exchanged in each different stroke is the same in the two engine cycles, the work statistics may be significantly different.

So it is important to first clearly set the specific conditions in which two engines (made with two different traps) are compared, and then what is the figure of merit, e.g. largest net work transfer, largest efficiency or smaller variance of the output.

4 Particle statistics and shape of the trap

We now focus on another aspect for which the shape of the trap plays a crucial role, and this is when we compare two engines with the same potential but with different types of working fluids. We consider one engine made with a gas of non-interacting, identical bosons and another with non-interacting, identical fermions. We will only consider traps made with a scale-invariant potential, such that during ideal quantum adiabatic processes the state remains thermal. We will also consider engine cycles at low enough temperatures such that the effects of the statistics will be more evident. The engine cycles will be determined solely by the temperatures of the baths and the parameters of the potential.

One key aspect of this study is the energy levels spacing due to the shape of the trap. For a fermionic gas at very cold temperatures, each fermion will occupy one of the lowest energy levels. The gap to excite such a gas is then due to the energy difference between the last occupied level and the first non-occupied level. Conversely for bosons, the relevant energy gap to excite the system is due to the energy between the lowest and the first energy levels, because all the bosons will be in the lowest energy level. For different traps the relevant gap for bosons could be larger or smaller than that of the fermions, and this will affect the performance of the engine cycle. For a harmonic oscillator (which is obviously a scale-invariant potential), all the energy levels are equally spaced and thus we do not expect a different behavior. In one dimension, for which there are no degeneracies, it is easy to compute analytically the work output and all the higher moments and they are identical whether the gas is made of non-interacting bosons or fermions [26].

For a trap in the form of an infinite square well, the separation between energy level increases for larger energy levels. It is thus expected that it is easier for the bosonic gas to exchange energy with the baths compared to the fermionic one, especially as the number of atoms is larger. This was clearly shown in the $T-S$ diagrams in [26]. For a different trapping potential, for example a linear potential $V(x) \propto |x|$ the distance between the energy levels becomes smaller as the energy level number increases. Hence a gas with many fermions will exchange more heat than the bosonic gas and this will result in a larger net work output [26].

In reality the comparison of the output of the engines with the two different working fluid cannot be fully understood by the analysis of the behavior at very cold temperatures. The ratio of the work outputs is a non-monotonous function of the temperature of the hot bath. This is due to the fact that the difference in the work output in the adiabatic stroke at hot temperature for fermions and bosons becomes large for the square well potential but goes to zero for the triangular potential.

We have so far discussed three potentials (harmonic, square and linear) for which the energy levels distance is a monotonous function of the energy level number. However, it is also possible to produce scale-invariant potentials with a non-monotonous distance between energy levels such as, for example, in double-well. In this case the ratio of the work output of the bosonic and fermionic engines is a non-monotonous function of the total number of atoms in the gas.

5 Conclusions

We have summarized some key aspects of quantum heat engines related to the geometrical shape of the trap confining the gas [25, 26]. First, we have discussed the types of traps for which a gas remains thermal when driven adiabatically. Then we discussed the comparison between heat engines made with the same gas but in traps of different shapes. We have concluded by examining how the comparison of working fluids with different work statistics is affected by the shape of the trap. It would be particularly interesting to further these studies examining other aspects. For instance the use of non-scale-invariant potentials and the entropy generated in them, and also processes which are not adiabatic [27]. An interesting study of non-adiabatic manybody engines was done in [28].

Engine cycles in traps of different shapes can be realized in various manner. One important candidate is the use of ions in Paul traps. Three important advantages include the fact that traps of different shapes can potentially be generated using segmented traps. Moreover it is possible to lower or increase the temperature of the system under study via side-band cooling/heating [29, 30]. Finally, it is possible to measure the occupation of the various energy levels thus giving us an insight into not only the average value of the energy and work, but also in their statistics, see for example [31]. A realization of an engine cycle with a single atom is discussed in [32].

Acknowledgments

The author is indebted to Y Zheng for his great contributions to our collaboration on quantum heat engines. This material is based upon work supported by the Air Force Oce of Scientific Research under award number FA2386-16-1-4041 and by the Singapore MOE Academic Research Fund Tier-2 project (Project No. MOE2014-T2-2-119, with WBS No. R-144-000-350-112).

References

1. Carnot S, Reflexions sur la puissance motrice du feu ´ (Bachelier, Paris), 1824.
2. Scovil H E D, Schulz-DuBois E O, *Phys Rev Lett*, 2(1959)262; doi:org/10.1103/PhysRevLett.2.262
3. Youssef M, Mahler G, Obada A.-S. F, *Phys Rev E*, 80(2009)061129;doi: org/10.1103/PhysRevE.80.061129
4. Linden N, Popescu S, Skrzypczyk P, *Phys Rev Lett*, 105(2010)130401; doi.org/10.1103/PhysRevLett.105.130401
5. Skrzypczyk P, Brunner N, Linden N, Popescu S, *J Phys A*, 44 (2011)492002; /doi.org/10.1088/1751-8113/44/49/492002
6. Teo C, Bissbort U, Poletti D , arxiv:1609.02294
7. Roulet A, Nimmrichter S, Arrazola J M, Scarani V, arxiv:1609.06011
8. Giazotto F, Heikkila T T, Luukanen A, Savin A M, Pekola J P, *Rev Mod Phys*, 78(2006)217; doi.org/10.1103/RevModPhys.78.217
9. Shakouri A, *Annu Rev Mater Res*, 41(2011)399-431; doi:10.1146/annurev-matsci-062910-100445
10. Dubi Y, Ventra M Di, *Rev Mod Phys*, 83(2011)131; doi.org/10.1103/RevModPhys.83.131

11. Sothmann B, Sanchez R, Jordan A N, *Nanotechnology*, 26(2015)032001; doi.org/10.1088/0957-4484/26/3/032001
12. Benenti G, Casati G, Meja-Monasterio C, Peyrard M, From thermal rectifiers to thermoelectric devices, in Thermal transport in low dimensions, S Lepri (Ed), Lecture Notes in Physics 921 (Springer, 2016).
13. Muhonen J T, Meschke M, Pekola J P, *Rep Prog Phys*, 75(2012)046501;doi:org/10.1088/0034-4885/75/4/046501
14. Seifert U, *Rep Prog Phys*, 75(2012)126001; doi:org/10.1088/0034-4885/75/12/126001
15. Koslo R, *Entropy*, 15(2013)2100-2128; doi:10.3390/e15062100.
16. Gelbwaser-Klimovsky D, Niedenzu W, Kurizki G, *Adv At Mol Opt Phys*, 64(2015)329-407; doi:org/10.1016/bs.aamop.2015.07.002
17. Vinjanampathy S, Anders J, *Contemporary Physics*, 57(2016)1-35; doi:org/10.1080/00107514.2016.1201896
18. Benenti G, Casati G, Saito K, Whitney R S, arXiv:1608.05595 [cond-mat.mes-hall].
19. Talkner P, Lutz E, Hänggi P, *Phys Rev E*, 75(2007)050102(R); doi:org/10.1103/PhysRevE.75.050102
20. Campisi M, Hänggi P, Talkner P, *Rev Mod Phys*, 83(2011)771-791; doi:org/10.1103/RevModPhys.83.771
21. Campisi M, Hänggi P, Talkner P, *Rev Mod Phys*, 83 (2011)1653; doi:org/10.1103/RevModPhys.83.1653
22. Deffner S, Jarzynski C, Campo Adolfo del, *Phys Rev X*, 4(2014)021013; doi: org/10.1103/PhysRevX.4.021013
23. Zheng Y, Campbell S, Chiara G De, Poletti D, *Phys Rev A*, 94(2016)042132; doi:org/10.1103/PhysRevA.94.042132
24. Xiao G, Gong J, *Phys Rev E*, 92(2015)012118; doi: org/10.1103/PhysRevE.92.012118
25. Zheng Y, Poletti D, *Phys Rev E*, 90(2014)012145; doi: org/10.1103/PhysRevE.90.012145
26. Zheng Y, Poletti D, *Phys Rev E*, 92(2015)012110; doi : org/10.1103/PhysRevE.92.012110
27. Zheng Y, Hänggi P, Poletti D, *Phys Rev E*, 94(2016)012137; doi: org/10.1103/PhysRevE.94.012137
28. Jaramillo J, Beau M, Campo A del, *New J Phys*, 18(2016)075019; doi:org/10.1088/1367-2630/18/7/075019
29. Leibfried D, Blatt R, Monroe C, Wineland D, *Rev Mod Phys*, 75 (2003)281; doi:org/10.1103/RevModPhys.75.281
30. Cirac J I, Blatt R, Zoller P, Phillips W D, *Phys Rev A*, 46(1992)2668; doi:org/10.1103/PhysRevA.46.2668
31. An S, Zhang J N, Um M, Lv D, Lu Y, Zhang J, Yin Z Q, Quan H T, Kim K, *Nature Physics* , 11(2015)193; http://www.nature.com/nphys/journal/v11/n2/abs/nphys3197.html
32. Roβnagel J, Dawkins S T, Tolazzi K N, Abah O, Lutz E, Schmidt-Kaler F, Singer K, *Science*, 352(2016)325-329; doi: 10.1126/science.aad6320

[*Received*: 13.12.2016; *accepted*: 25.12.2016]

Dario Poletti

Dario Poletti is Assistant Professor at the Singapore University of Technology and Design (SUTD). He received a double Master degree in Engineering from Politecnico di Milano and Ecole Centrale Paris. He then obtained a Joint Ph.D. in Physics from the National University of Singapore and the Australian National Unversity. **Dr Poletti** then researched at the Centre for Quantum Technologies, at the Ecole Polytechnique and at the University of Geneva before joining SUTD in 2012. His research focuses on manybody quantum mechanics with applications to energy conversion and transport.