Single Atom Heat Engine

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Abstract

The concept of a Single-atom heat engine represents a fundamental exploration of the thermodynamics of heat engines at the nanoscale. Heat engines convert thermal energy into mechanical energy, generally containing large numbers of atoms or molecules. In this heat engine, a single calcium ion is used as the working substance of the heat engine, confined that ion in a linear paul trap but tapered the geometry of the linear to funnel-shaped. This single atom is brought into contact with a hot reservoir, which is nothing but electric field noise. The atom absorbs energy from the hot reservoir, performs work, and releases it into the cold reservoir. Ions get driven in a thermodynamical stirling cycle, thus functioning as a heat engine.

The work generated in that thermodynamical process can be extracted and stored also. They evaluated the output power and efficiency of that single atom heat engine, power can reach up to $p = 3.4 \times 10^{-22} j/s$ and efficiency $\eta = 0.28\%$. This was the first experimental realization of a single-atom heat engine, before that it was not even clear whether such a tiny engine could work or not. This can inspire and initiate future thermodynamic experiments on heat engines with better efficiency and power.

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1 Introduction

In 2015, a team of Experimental physicists led by Johanesse Roßnagel at the University of Mainz in Germany built the smallest working heat engine consisting of only one atom. Back in 2014, Johanesse Roßnagel published a paper in which he talked about this Singl-Atom heat engine, and next year, for the experimental visualization of the Single-atom heat engine, they built it, and it works exactly as he said it would. The engine has the same working principle as our normal combustion engine, which is used in cars or any other vehicle, and follows the same four strokes: expansion, cooling, contraction, and heat addition.

In the Experimental realization of a Single-atom heat engine, they trapped a calcium ion in a funnel-shaped ion trap in which they used electric field noise to heat the atom, laser cooling to cool the atom, and because of this heating and cooling, the atom starts moving back and forth inside the paul trap and subjected to a thermodynamical cycle. This Single-atom heat engine can generate power of $p = 3.4 \times 10^{-22} \frac{j}{s}$ with efficiency of up to y $\eta = 0.28\%$. Although the efficiency and power is very low, the goal of this experimental realization of the single-atom heat engine is to get new insight into the fundamental science of heat engine, and It was never meant to make an engine of very high efficiency.

2 Heat Engine

A heat engine is a device that converts the difference in thermal energy of the sink (cold reservoir) and source (heat reservoir) into some mechanical energy. In simple words, Heat Engines convert heat into work.

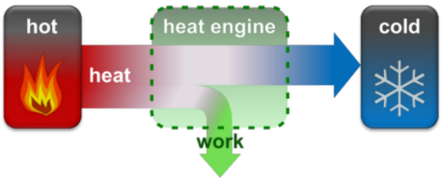


Figure 1: Heat Engine,ref-2

$$Efficiency = \frac{WorkOutput}{HeatInput}$$

$$\eta = \frac{W}{Q_i n}$$

2.1 Laws of Thermodynamics

2.1.1 Zeroth Law

In a system of three bodies, if two bodies, A and B, are in thermal equilibrium with C, then it is stated that they (A and B) will also be in equilibrium with each other.

2.1.2 First Law of Thermodynamics

The First Law of Thermodynamics Is the reflection of energy conservation, which states that the heat absorbed or released is equal to the change in internal energy and work.

$$\Delta \mathrm{Q} = \Delta \mathrm{U} + \Delta \mathrm{W}$$

where $\Delta \mathrm{Q} = TdS$ denotes the net heat of the system and $\Delta \mathrm{w} = pdv$ denotes the net amount of the work done by the system.

2.1.3 Second Law of Thermodynamics

It is a phenomenological law which explain why some process does not occur spontaneously. Only those process occur in nature in which the entropy of the isolated system either increases or remain constant.

$$\Delta \mathrm{S} \geq 0$$

Where, **Entropy** is the quantity to measure the randomness or disorder of the system, it was introduced by Rudolf Clausius to represent microscopic changes by a macroscopic quantity.

$$ds = \frac{dQ}{T}$$

2.1.4 Third Law of Thermodynamics

If $T \rightarrow 0$ then the contribution to entropy from all component of the system tends to zero.

$$T \rightarrow 0 \implies S \rightarrow 0$$

This law, also known as the Nernst heat theorem or the unattainability principle, implies that as a system reaches absolute zero temperature (0 Kelvin), its entropy approaches a minimum possible value, and it becomes perfectly ordered. Additionally, the statement often emphasizes that it is practically impossible to reach absolute zero in a finite number of steps.
The third law of thermodynamics has important implications for the behaviour of matter at low temperatures and is particularly relevant in the study of phenomena such as phase transitions and the properties of materials near absolute zero.

3 Stirling Cycle

There are several Thermodynamic cycles we know and read in our academics like the Carnot Cycle, Otto Cycle etc, but the one which has been used in our Single-Atom heat engine is the Stirling Cycle. Stirling Cycle is a thermodynamical cycle consisting of four processes, two isothermal and two isochoric processes, It was developed in 1816 by Robert Stirling. The key difference between Carnot and Stirling is that in place of two isoentropic processes, two isochoric processes are used. In a Stirling cycle, the working agent is permanently coupled with one of the heat engines. Therefore, the two isoentropic processes are replaced by the two isochoric processes.

Process	Change in Internal energy	Heat Interaction	Work Interaction
Process(c) 1-2	0	RT1 ln(V2/V1)	RT1 ln(V2/V1)
Process(d) 2-3	Cv(T1-T2)	Cv(T1-T2)	0
Process(a) 3-4	0	RT2 ln(V4/V3)	RT2 ln(V4/V3)
Process(b) 4-1	Cv(T1-T2)	Cv(T1-T2)	0

The Table simply shows the value of quantities like heat energy absorbed or released, work done and internal energy of the system calculated using the first and second law of thermodynamics.

The Four processes involved in our sterling cycle are the following:-

(a) Isothermal compression: Cold gas is compressed isothermally, temperature remains the same, and work is done on the gas.

(b) Hot Isochore: Cold gas is transferred to the hot reservoir; no work is done on or by the system by keeping it at constant volume.

(c) Isothermal expansion: Work done by the gas; the volume gets expanded. To maintain the temperature and not to cool down the equal amount of heat from the hot reservoir.

(d) Cold isochore: Volume remains the same; hence, no work is done on or by the system, and the system is transferred back to the cold reservoir by losing a quantity of heat.

$$\begin{aligned}\eta &= \frac{work\ output}{heat\ input}\\ &= \frac{R(T_2 - T_1)\ln\left(\frac{v_2}{v_1}\right)}{C_v(T_2 - T_1) + RT_2\ln\left(\frac{v_2}{v_1}\right)}\end{aligned}$$

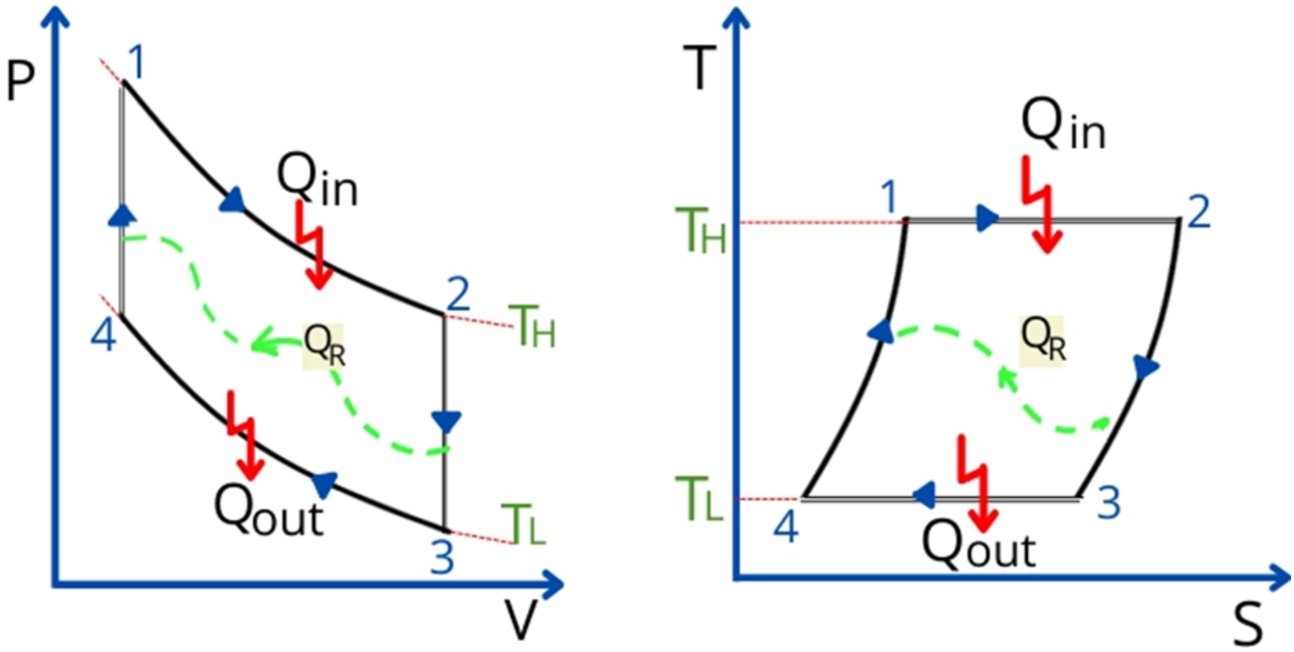


Figure 2: P-V and T-S curve of Stirling cycle

and since the sterling cycle is a regenerative type of cycle, the heat output from process 2→3 is used in the process of heat input in process 4→1, thus if we remove the part $C_v(T_2 - T_1)$ from the efficiency equation and also in these two isochoric process $v_2 = v_3$ and $v_4 = v_1$, then efficiency will be similar to the equation of Carnot cycle.

$$\eta = 1 - \frac{T_1}{T_2}$$

4 Dopler Cooling

Doppler Cooling is one of the methods of laser cooling to cool the atom, ion or molecule with the help of a laser by slowing it down. The cooling process takes advantage of this Doppler shift. Laser beams are tuned slightly below the natural frequency of an atomic transition. Atoms moving towards the laser see the light as blue-shifted, and those moving away see it as redshifted.

Temperature is the measure of thermal energy in the form of random motion of the particles. The random motion will be high if the temperature is high, and the random motion of the particles will be less if the temperature is low. Hence, to cool something, we need to slow it down or make a device that can hold all the particles.

Doppler effect is used in favour of laser cooling. A change in the frequency(wavelength) of light due to relative motion between source and observer is called the Doppler effect.

$$\nu = \frac{\nu_0\sqrt{1 - \frac{v^2}{c^2}}}{1 - \frac{v\cos\theta}{c}}$$

if I take the approximation cv then we will get a very simple formula for the Doppler shift in frequency.

$$\nu = \nu_0\left(1 - \frac{\nu}{c}\right)$$

from this equation we can see if the particle moves away from the source,$\rightarrow$ light is Red-shifted and if the particle moves toward the source,$\rightarrow$ light is Blue-shifted.

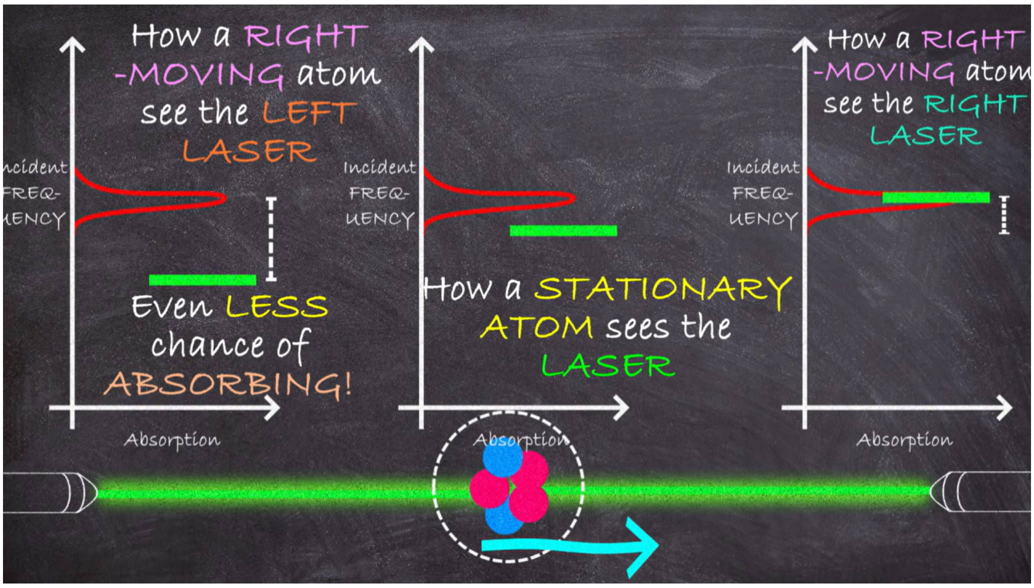


Figure 3: Doppler cooling,ref-6

In Doppler cooling, a gas of atoms is detuned to a frequency lower than the atomic frequency for a stationary atom. When an atom is moving towards a laser, it sees it as blue-shifted and absorbs the photons, gaining a kick backward. Conversely, if it's moving away from a laser, the red-shifted frequency prevents absorption. This process, based on the Doppler effect, selectively cools atoms in the direction opposing their motion, effectively limiting their speed. Doppler cooling, also known as optical molasses, achieves temperatures much colder than those attainable with Zeeman cooling, trapping atoms through constant scattering of photons and inducing a random walk of motion. Notably, Steven Chu was instrumental in demonstrating optical molasses and was awarded the Nobel Prize in Physics in 1997 for his contributions to laser cooling techniques.

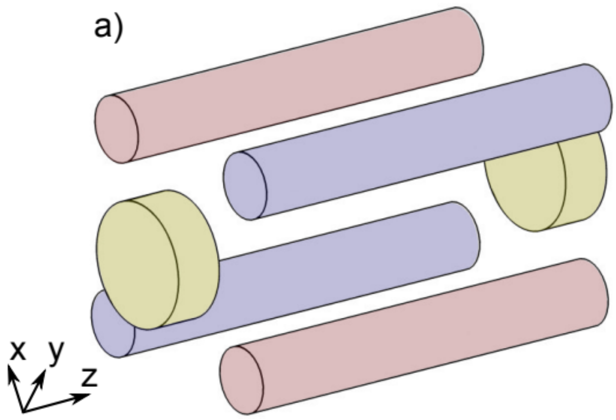
5 Ion Trapping

Ion trapping is a powerful and versatile technique used in experimental physics to confine and manipulate ions using electromagnetic fields. There are several methods of ion trapping, with the most common being radiofrequency (RF) and Paul traps.

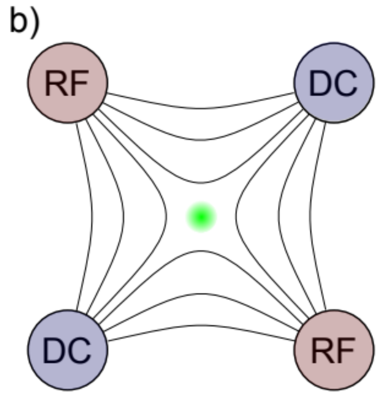
5.1 Linear Paul Trap

In a Linear Paul trap, a rapidly oscillating electric field is applied to trap ions. The ions experience a pseudopotential that confines them to the centre of the trap.

The geometry of linear Paul trap, featuring two grounded or biased endcap electrodes (yellow) and four elongated electrodes (two red, two grounded or biased with DC voltage). The endcaps create static electric fields, while the oscillating voltage applied to the red electrodes generates a dynamic field, collectively forming a pseudopotential that confines ions. This trapping method, notable for its application in quantum computing and precision spectroscopy, enables precise control over individual ions by manipulating the dynamic and static electric



(a) Linear Paul Trap configuration,ref-2



(b) Oscillating electric field trapping the ion in the centre of the Linear Paul Trap,ref-2

fields. The stability and versatility of this ion trap make it a valuable tool in experimental physics.

In order to satisfy the Laplace equation $\delta^2\phi = 0$ as there is no dielectric used in the Linear Paul trap, a combination of both static and oscillating electric fields is needed, because of the symmetrical arrangement of four electrodes leads to an electric quadrupole field.

The Oscillating potential,

$$V_{rf} \propto \frac{U_{rf}}{r_0^2} \sin{(\Omega_{rf} t)}(x^2 - y^2)$$

Where U_{rf} is the amplitude of oscillating voltage at radio frequency Ω_{rf} and r_0 is the distance of the electrode from the trap axis(the line exactly at the centre of the linear Paul trap where the ion gets trapped), now if we solve the differential equation of, equation of motion for this oscillating potential, we will get a formula for the trap frequency but that's not what we want the trap frequency to be only depended on one direction so that with the help of the ICCD camera we can get the position of the ion and from that we can calculate the trap frequency.

5.2 Funnel Shaped Paul Trap

A normal linear Paul trap was not used in that experiment, they tapered the linear Paul trap and used a funnel-shaped ion trap by bending away the elongated electrodes by 10 degrees. This is beneficial for their experiment in two ways:- first, the radial confinement is not uniform in the funnel-shaped Paul trap; radial confinement will keep decreasing from left to right. Second, when we calculate radial frequency using the equation of motion in the case of a funnel-shaped ion trap. Which only depends on the axial position Z, hence with the value of Z we can get the value of radial frequency because other things are constant and known.

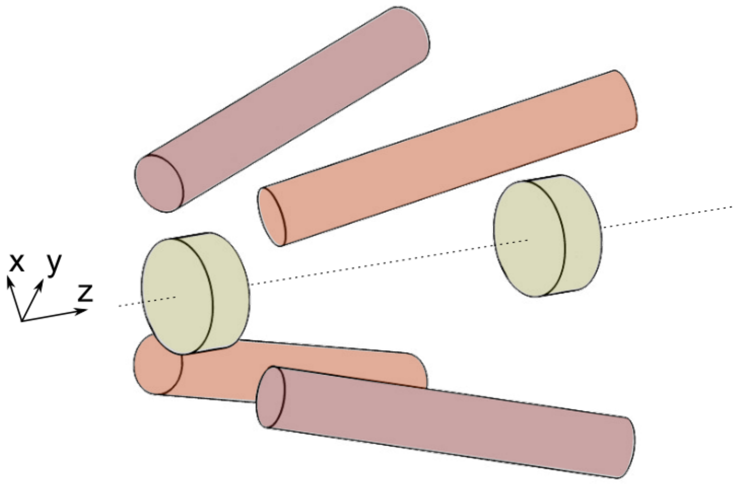


Figure 5: Funnel Shaped Paul Trap,ref-2

Due to the tapering of the linear Paul trap to a funnel-shaped Paul trap, the radial confinement remains the same but the confinement along the Z-axis will vary as the confinement of ion keeps increasing from left to right along the Z-axis, the modified oscillating potential,

$$V_{rf} \propto \frac{U_{rf}}{r_0^2} \sin{(\Omega_{rf} t)} (x^2 - y^2) + \frac{U_{dc}}{Z_0^2} z^2$$

now if we solve the differential equation, of the equation of motion due to this modified oscillating potential, we get the expression of radial trap frequency which is nothing but the only function of position z and the other parameters are constant.

$$\omega_{x,y} = \frac{\omega_{0x,0y}}{1 + Z \tan\theta / r_0}$$

5.3 The Calcium Ion

In Paul-trap experiments for laser cooling, earth-alkali ions, specifically Ca^+, are preferred due to their simplified electronic ground-state configuration analogous to Argon and the absence of nuclear spin, resulting in no hyper-fine structure. The ions' level structure with only fine structure including $4s^2S_{1/2}$,$3d^2D_{3/2}$, and $4p^2P_{1/2}$ is crucial. The intricate energy level scheme is condensed to a manageable three-level system to streamline the experimental setup. This choice facilitates the reduction of experimental complexity and optimization of conditions for laser cooling in Paul traps.

6 Working Cycle of Single-Atom Heat Engine

The classical description of the ion is more suitable than the quantum mechanical description because the thermal energy evolve in the process is much high compared to the energy of quantized harmonic oscillator($K_B \gg \hbar\omega_r$).

Thermal processes, involving both heating and cooling, result in the ion adopting thermal states characterized by varying temperatures T. This leads to a time-averaged spatial distribution described by the expression

$$\zeta(r,T) = \frac{q}{2\pi\sigma^2(T)} \exp\left\{-\frac{(r-r_0)^2}{2\sigma^2(T)}\right\}$$

Where $\sigma(T)$ is the time-averaged width of Gaussian probability distribution can be defined as:

$$\sigma(T) = \sqrt{\frac{K_B T}{m\omega_r^2}}$$

where m is the mass of the ion, ω_r is the radial trapping frequency of the ion and K_B is the Boltzmann constant.
In the single-atom heat engine, On one side we need one source to heat our single ion, electric field noise will play the role of source in our experiment and on the other side one sink to cool down our single ion, the laser will play the role of sink in our experiment.

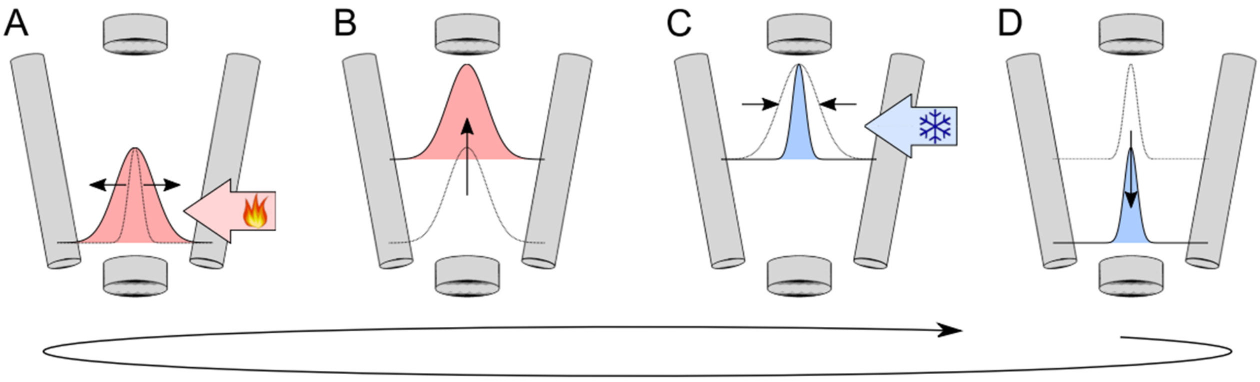


Figure 6: All the four processes involve in our Single-Atom heat engine,ref-2

1. **Hot isochoric process**$(\omega_2, T_1 \rightarrow \omega_2, T_2)$:- Initially, the cold calcium ion is heated, and the width of the probability distribution expands, no work is done in this process, the frequency remains same.

2. **Isothermal expansion** $(\omega_2, T_2 \rightarrow \omega_1, T_2)$:- as a result of process A ion moves along the Z axis to a weaker radial confinement, that is one of the reasons the linear paul trap is tapered to funnel-shaped paul trap, work done on the system, the temperature remains same and the frequency changes.

3. **Cold isochore** $(\omega_1, T_2 \rightarrow \omega_1, T_1)$:- Calcium ion cooled down to the initial temperature, cooling the ion reduces the radial width of its probability distribution, no work is done or by the system.

4. **Isothermal compression** $(\omega_1, T_1 \rightarrow \omega_2, T_1)$:-Due to the restoring force of the axial potential, ion move back to its initial position.

7 Experimental Implementation of Single-Atom Heat Engine

For the experimental implementation of a single-atom heat engine, they used the funnel-shaped Paul to trap the ion at the centre of the Paul trap and the opposing noise signals were supplied to the outer electrodes, to generate electric field noise without affecting the trap frequency and this external electric field noise to heat the ion from one side and used the laser to cool the atom from the other side, and because of this heating and cooling of calcium ion in the funnel-shaped paul trap, the ion starts moving back and forth inside the paul trap and subjected to a thermodynamic cycle.

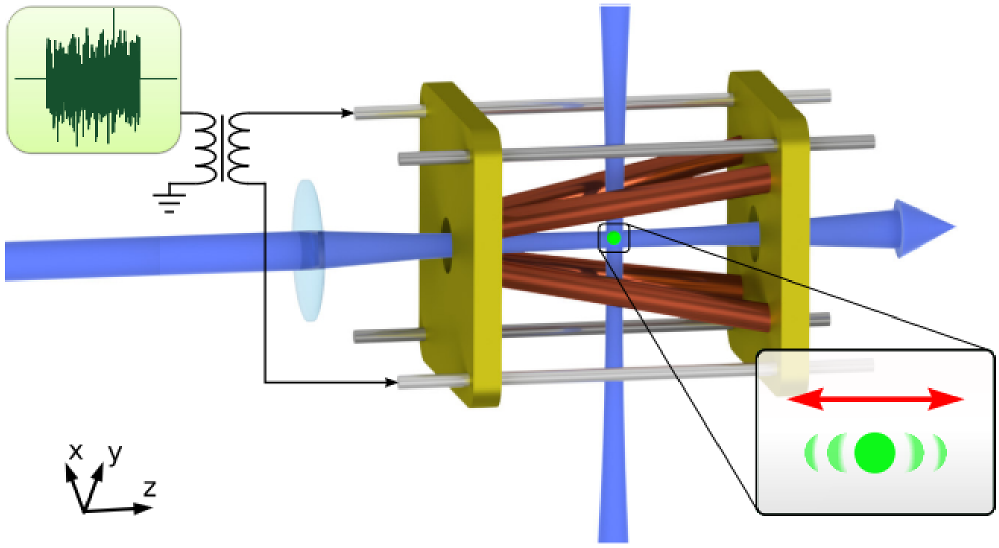


Figure 7: Experimental setup of Single-Atom heat engine, Calcium ion(green) get trapped in the middle of the funnel-shaped paul trap,ref-1

Using this experimental setup, they determine the position of the ion inside the funnel-shaped Paul trap using an ICCD(intensified charge-coupled device) camera as a function of time, by doing this now we the position of the ion(z values), the position of the ion is determined by the more than 200,000 of images of the ion at each time step.

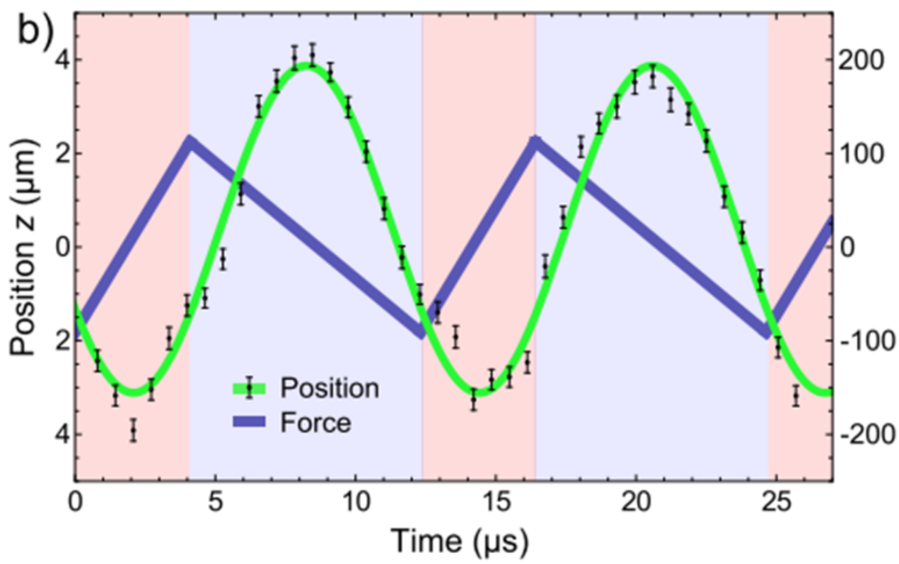


Figure 8: Position vs time of calcium ion,ref-1

The benefit is that now we know the position(Z values) of the calcium ion inside the funnel-shaped ion trap, and with the positions of the ion, we can calculate the trap frequency, because of tapering of the Paul trap, the trap frequency is the function of position only and other parameters $\omega_{0x,0y}$,θ and r_0 are constant and already known,

$$\omega_{x,y} = \frac{\omega_{0x,0y}}{1 + Z\tan\theta/r_0}$$

The laser beam used to cool the calcium ion was of wavelength 397nm, $r_0 = 1.1mm$ is the radial extent of trap at z=0, $\theta = 0$, $\omega_{0x,0y} = 450kHz$ and the radial trap frequency $w_{x,y}$ diminishes along the z-direction.

7.1 Thermodynamical Cycle

The change in trap frequency is directly deduced directly from the Z position of the ion and the relative phonon number $\langle n \rangle$ is determined from the separate measurements it was not the part of this experiment and now if plot $\{\omega_r, n_r\}$ curve it will give us the thermodynamical cycle of our experiment which is already discussed in the above sections.

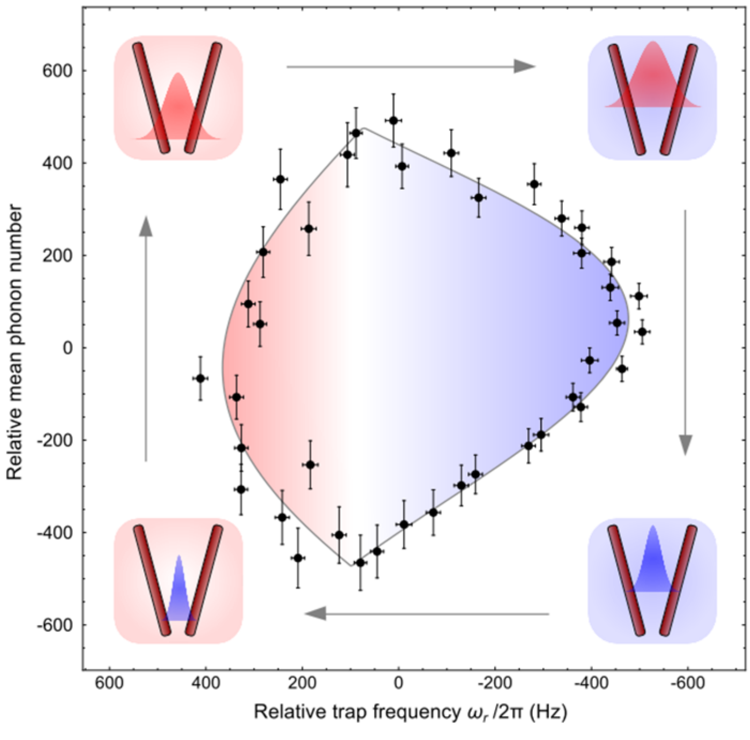


Figure 9: $\{\omega_r, n_r\}$ curve,ref-1

Now to calculate the power, efficiency and work of the thermodynamical cycle we need to transform this curve to T-S or P-V curve.
We can calculate the temperature of the experiment corresponding to relative phonon number using:

$$n = \frac{K_B T}{\hbar\omega_r}$$

to calculate the entropy of the system we can use:

$$S = k_B \left(1 + \ln \frac{K_B T}{\hbar \omega_r}\right)$$

using above equations now we can transform our curve $\{\omega_r, n_r\} \rightarrow \{T, S\}$ curve.

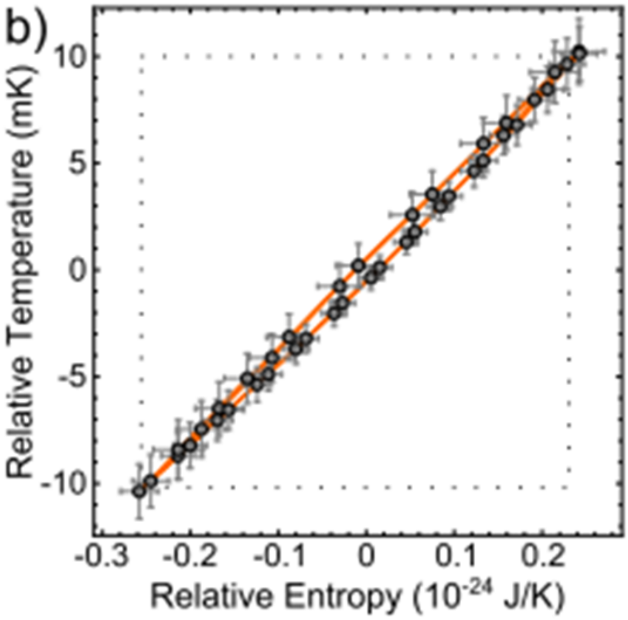


Figure 10: Transformed $\{T, S\}$ curve

7.2 Power and Efficiency

Now we have the T-S curve of our single-atom heat engine we can easily calculate the Work as we know the area inside the curve shows the work done, just by looking at the curve we can clearly say that the work done is much less in comparison to conventional heat engines of car or other vehicles.

$$\eta = \frac{W}{Q}$$

Where, $Q = \int T ds$, and They performed this experiment several times with different temperature differences and calculated the power and efficiency of the cycle. The maximum efficiency they get is 0.28% and the maximum power was $p = 342 \times 10^{-24} j$.

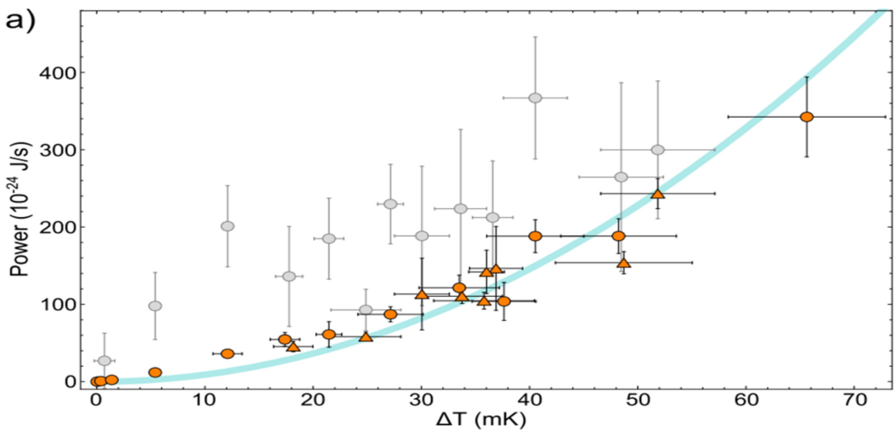


Figure 11: powr vs $\Delta T curve, ref - 1$

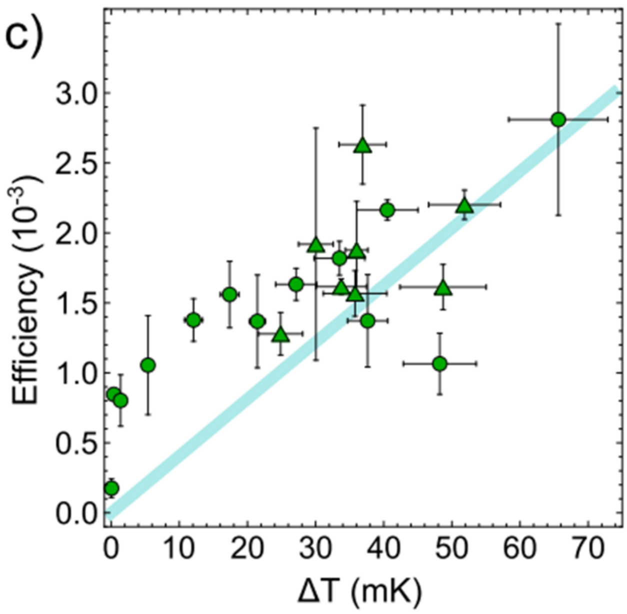


Figure 12: Efficiency vs ΔT curve, ref-1

By using the Curzon-Ahlborn formula if we calculate the efficiency of a single-atom heat engine at maximum power, we can do this by using the formula:

$$\eta = 1 - \sqrt{\frac{T_1}{T_2}}$$

They get the efficiency $\eta = 1.9\%$ although we know that the efficiency and power of our single-atom heat engine is much less compared to the conventional heat engine, but this experiment was never meant to make a futuristic heat engine and revolutionise the sector of heat engine, the primary aim of this experiment was to study the thermodynamics of such a small engine before this experiment it was not even confirmed that the engine with such a small no of the particle(one atom) can even work.

8 Future Perspective and Potential Application

Single-Atom heat pump by inverting the thermodynamic cycle of the engine, absorbing heat from a cold reservoir and releasing it to a hot reservoir. This process increases the temperature difference between the two reservoirs. Driving the ion in this manner requires an external supply of work since the heat pump moves heat against the direction of spontaneous heat flow, consuming energy. The practical application of nanoscopic heat pumps holds significant importance for future technologies, especially considering the challenges associated with heat production and dissipation in nanodevices with limited heat capacities and the need to operate in isolation from other systems.

One of the primary goals of this experiment was to know about the thermodynamics of a single particle and delve into the **quantum regime**, there are several theoretical investigations have been done on quantum heat engine, but till now there is not any experimental realization of quantum heat engine, therefore it is unclear what can be the practical efficiency of the heat engine, maybe it can break the boundation of Curzon-Ahlborn efficiency and come up with efficiency beyond the limits of classical heat engine. Our first experimental realized single-atom heat engine has the potential to operate in a quantum regime.

For sure our single-atom heat engine can't be used directly in the car or any future technology, but it gives us so much information about the thermodynamics of a single particle and shows that the single particle follows the same laws as a large number of particles in other engines of car or vehicles and can help us in fundamental research of future technologies, also it can have so many applications in nanotechnologies and microelectronics.

9 Conclusion

In the groundbreaking experiment, they successfully realized a heat engine operating at the fundamental limit of a single atom. Utilizing a single trapped ion as the working agent, they conducted experiments to investigate single-particle thermodynamics. Employing a Stirling cycle, observed the conversion of thermal and undirected excitations into coherent and directed motion in the ion. The exceptional versatility of the trapped ion system enabled direct measurements of key engine features, including thermodynamic cycles, power output, and efficiency. Although the efficiency remains comparatively low compared to the Curzon-Ahlborn efficiency, our system exhibits remarkable relative output power comparable to macroscopic engines, despite a vast difference in particle numbers. This work establishes that classical thermodynamics principles can be applied to our single-atom system, with the caveat that the concept of temperature necessitates careful consideration. Our classical device provides a robust platform for future experiments, exploring topics such as thermal fluctuations of work and heat, machines coupled to non-thermal reservoirs, nanoscopic refrigerators, and quantum heat engines, as detailed in specific sections.

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