Quantum Dot Heat Engine Review

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1 Introduction

Due to the discrete nature of their density of states, quantum dots display the ability to serve as a nearly ideal energy filter. When used in combination with two electrons reservoirs (hot and cold), they allow for very efficient thermoelectric energy conversion and form a quantum dot heat engine.

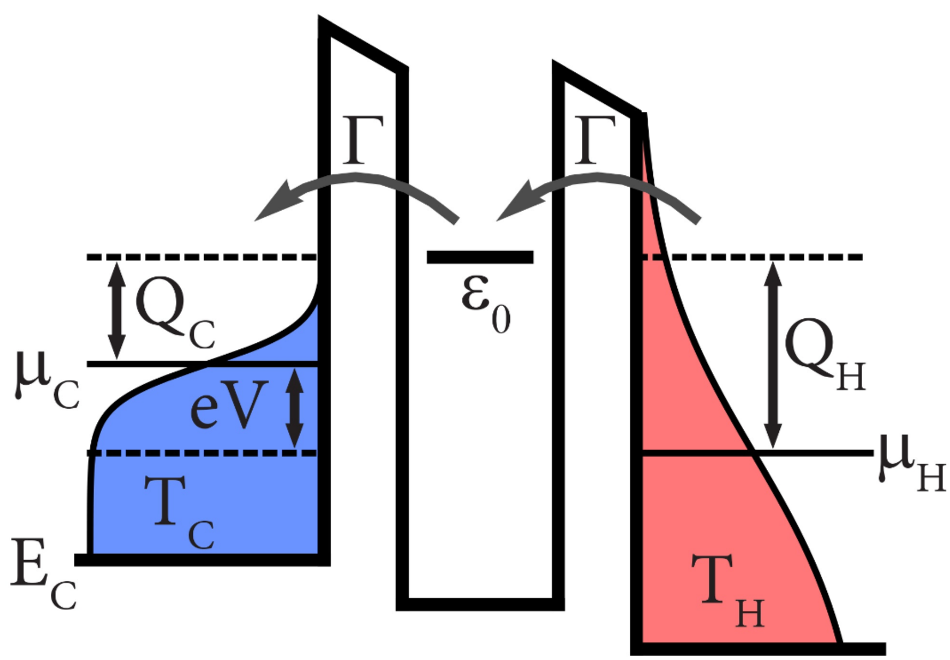

Figure 1: Schematic of a Quantum Dot Heat Engine showing the quantum dot connected to hot and cold reservoirs. *Source:* [1]

2 Key Components of a Quantum Dot Heat Engine

2.1 Quantum Dot (QD)

Quantum dots (QDs) are nanoscale semiconductors that confine electrons in all three spatial dimensions. The confinement forces their energy levels to be discrete, usually denoted $\{\varepsilon_0, \varepsilon_1, \varepsilon_2, \ldots\}$. These levels act as an energy filter: only electrons whose energies match an ε (or lie close to it) can tunnel through.

2.2 Reservoirs

2.2.1 Hot Reservoir (T_H, μ_H)

The hot reservoir serves as a supply of higher-energy electrons for the QD. It is characterized by a high temperature T_H and a low chemical potential μ_H.

2.2.2 Cold Reservoir (T_C, μ_C)

The cold reservoir receives the electrons that have lost energy from the QD. It is characterized by a low temperature T_C and a high chemical potential μ_C.

2.3 Tunnel Coupling (Γ)

Electrons can tunnel between the QD and each of the reservoirs at a characteristic rate Γ. This rate depends on the tunneling Hamiltonian and the density of states in the reservoirs.

2.4 Voltage Bias (ΔV)

A bias voltage V is applied in the two reservoirs. This creates a chemical potential difference: $eV = \mu_C - \mu_H$, where e is the electron charge. This difference quantifies the output of the engine.

3 Why Use a Quantum Dot?

3.1 Quantum Confinement And Discrete Levels

When electrons are confined in a small region of space, referred to as a "box," the allowed energies become quantized and given by the formula:

$$E_n \propto \frac{n^2}{L^2}$$

Here L is the size of the quantum dot and n is an integer (e.g., $n = 1, 2, 3, \ldots$). As L becomes extremely small (on the order of a few nanometers), the energy spacing ΔE between the quantized levels becomes large, making the energy levels easily distinguishable.

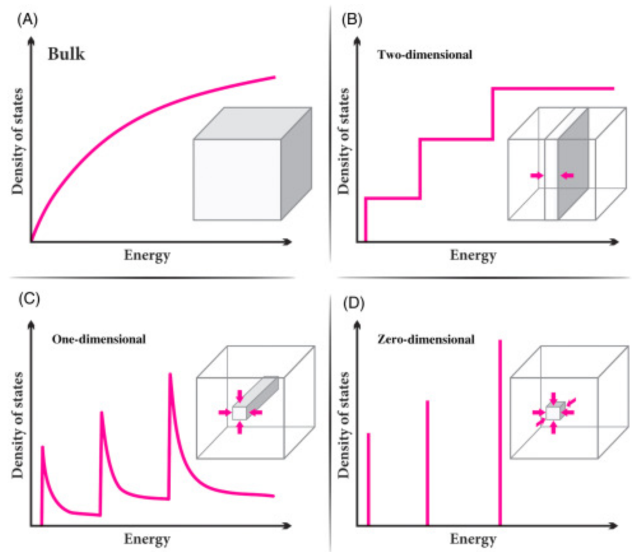

Figure 2: Schematic of the evolution of the energy levels depending on the confinement. *Source:* [3]

3.2 Role as an Energy Filter

The single (or dominant) QD level ε_0 picks out only those electrons whose energy matches ε_0. If the QD is weakly coupled to its reservoirs, the density of states $\rho(E)$ can be approximated by a sharp peak:

$$\rho(E) \approx \delta(E - \varepsilon_0).$$

This "δ-function" shape means only electrons with $E \approx \varepsilon_0$ can pass, thus allowing for efficient transport.

4 The Role of the Chemical Potential μ

4.1 Definition of μ

Thermodynamically, the chemical potential is:

$$\mu = \left(\frac{\partial U}{\partial N}\right)_{S,V},$$

where U is internal energy and N is particle number. Physically, μ is the energy cost (or gain) to add one more particle to the system.

4.2 Why μ Is Important

The chemical potential μ determines how electrons flow between the QD and the reservoirs. In the quantum dot heat engine $\mu_C > \mu_H$, this effectively drives the transport of electrons "uphill" in energy, against the voltage difference, allowing energy harvesting.

4.3 Quantum Transport Modes

- **Equilibrium:** If two reservoirs have $\mu_H = \mu_C$ and $T_H = T_C$, then there is no net current. Electrons can effectively move between reservoirs without needing a driving force.
- **Non-equilibrium:** A difference $\mu_C \neq \mu_H$ drives electron flow, fundamental to heat-engine operation.

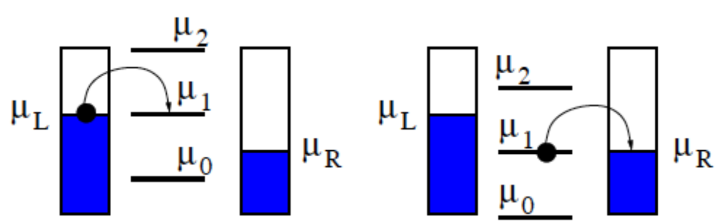

Figure 3: Illustration of an electron moving from the left reservoir μ_L to the right μ_R by tunneling through a quantum dot. *Source:* [2]

5 Basic Operation of the QD Heat Engine

We consider a single resonant level ε_0 in the QD, which is coupled to a hot reservoir (T_H, μ_H) and a cold reservoir (T_C, μ_C).

5.1 Electron Flow Steps

5.1.1 Absorption from Hot Reservoir

A high-energy electron from the hot reservoir tunnels into the QD, carrying energy ε_0. A "quantum of heat" gets therefore removed from the hot reservoir, approximately

$$Q_H = \varepsilon_0 - \mu_H \quad \text{if} \quad \varepsilon_0 > \mu_H.$$

5.1.2 Energy Conversion

The electron in the QD now has energy around ε_0. Due to the difference in chemical potential between the reservoir, the electron needs to have lower energy to tunnel to the cold reservoir. This energy difference can be converted into work. The work extracted per electron is directly related to eV, where

$$eV = \mu_C - \mu_H.$$

5.1.3 Deposition into Cold Reservoir

The electron eventually goes into the cold reservoir and deposits an amount of heat:

$$Q_C = \varepsilon_0 - \mu_C,$$

5.1.4 Energy Conservation

The heat taken from the hot reservoir minus the heat delivered to the cold reservoir appears as electrical work:

$$Q_H = Q_C + eV.$$

6 System Hamiltonians and Tunneling

The total Hamiltonian of the above picture is given by:

$$H = H_{\text{QD}} + H_{\text{res}} + H_{\text{tun}}$$

6.1 Quantum Dot Hamiltonian (H_{QD})

$$H_{\text{QD}} = \sum_{\sigma} \epsilon_\sigma n_\sigma + E_C n_\uparrow n_\downarrow$$

- ϵ_σ: Single-particle energy for an electron with spin σ.
- $n_\sigma = d_\sigma^\dagger d_\sigma$: Number operator for electrons in the quantum dot with spin σ.
- E_C: The energy cost from the double occupation of the quantum dot due to electron-electron interactions.

6.2 Reservoir Hamiltonians (H_{res})

$$H_{\text{res}} = \sum_{k,\sigma,r} \omega_{k,\sigma,r} c_{k,\sigma,r}^\dagger c_{k,\sigma,r}$$

- $\omega_{k,\sigma,r}$: Energy of a state in reservoir r with quantum numbers k and σ.
- $c_{k,\sigma,r}^\dagger$ and $c_{k,\sigma,r}$: Creation and annihilation operators for the reservoir.

6.3 Tunneling Hamiltonian (H_{tun})

$$H_{\text{tun}} = \sum_{k,\sigma,r} t_{k,\sigma,r} d_\sigma^\dagger c_{k,\sigma,r} + \text{h.c.}$$

- $t_{k,\sigma,r}$: Amplitude for tunneling between the quantum dot and reservoir r.
- $d_\sigma^\dagger$, $c_{k,\sigma,r}^\dagger$: Creation operators for the dot and reservoir, respectively.
- h.c.: Hermitian conjugate.

6.4 Tunneling Rates and Broadening

$$\Gamma_r = \frac{2\pi \nu_r |t_{k,\sigma,r}|^2}{\hbar}$$

- ν_r: Density of states of the reservoir.

7 Currents and Observables

7.1 Charge Current

The charge current I_r gives the rate at which particles leave a reservoir. It is the time derivative of the particle number in reservoir r:

$$I_r = -\frac{dN_r}{dt} = -i[H, N_r],$$

where:

- $N_r = \sum_{k,\sigma} n_{k,\sigma,r}$: Particle number operator in reservoir r,
- H: Total Hamiltonian of the system.

Using charge conservation it can also be expressed as:

$$I_r = -\frac{i}{2}\mathrm{Tr}\left[L_N^+ W_r\right],$$

where:

- L_N^+: Commutator super-operator for the particle number,
- W_r: Kernel describing the tunneling processes specific to reservoir r.

7.2 Heat (Energy) Current

The heat current $J_{Q,r}$ quantifies the heat flow from a reservoir. It is given by:

$$J_{Q,H} = J_{E,H} - \frac{\mu_H}{e} I_H,$$

where:

- $J_{E,H}$: Energy current from the hot reservoir,
- μ_H: Chemical potential of the hot reservoir,
- I_H: Charge current leaving the hot reservoir.

The energy current $J_{E,H}$ is calculated by:

$$J_{E,H} = i\,\mathrm{Tr}\left[L_{H_{\mathrm{QD}}}^+ W_H \rho_D\right] - i\,\mathrm{Tr}\left[W_\Gamma, H\right]\rho_D,$$

where:

- W_H: Tunneling processes kernel at the hot reservoir,
- ρ_D: Reduced density matrix of the quantum dot,
- W_Γ: Higher-order tunneling contributions.

8 Power and Efficiency

8.1 Power

The thermoelectric power output (P_{th}) of the quantum dot heat engine is given by:

$$P_{\text{th}} = -I_{\text{th}} V,$$

where:

- I_{th}: Thermoelectric current (thermocurrent),
- $V = \frac{\mu_C - \mu_H}{e}$: Voltage difference between the chemical potentials of the reservoirs.

8.2 Heat Input

The heat extracted from the hot reservoir is roughly:

$$J_{\text{Q},H} \approx I \times (\varepsilon_0 - \mu_H)$$

for a single dominant level ε_0.

8.3 Efficiency

The engine efficiency η is:

$$\eta = \frac{P}{J_{\text{Q},H}} = \frac{I\,(\mu_C - \mu_H)/e}{I\,(\varepsilon_0 - \mu_H)}$$

In principle, if ε_0 is exactly aligned so that electrons enter from the hot side at ε_0 and exit to the cold side at ε_0, you can approach Carnot efficiency:

$$\eta_{\text{Carnot}} = 1 - \frac{T_C}{T_H}$$

However, perfect alignment and infinitely narrow levels produce zero power (no net current). A compromise in level broadening Γ yields finite power at lower efficiency (akin to the Curzon–Ahlborn limit).

9 References

References

[1] Josefsson, M., Svilans, A., Burke, A. M., Hoffmann, E. A., Fahlvik, S., Thelander, C., Leijnse, M., & Linke, H. (2017). *A quantum-dot heat engine operating close to the thermodynamic efficiency limits*. arXiv:1710.00742.

[2] Coulomb blockade in metallic islands and quantum dots. Retrieved from https://www.ftf.lth.se/fileadmin/ftf/Course_pages/FFF042/Coulomb_blockade.pdf.

[3] Zultak, J. (2018). *Optoelectronics of new two-dimensional semiconductors*. Retrieved from ResearchGate. DOI: 10.13140/RG.2.2.22858.59845.