

Controlling heat and particle currents in nanodevices by quantum observation

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We demonstrate that in a standard thermo-electric nanodevice the current and heat flows are not only dictated by the temperature and potential gradient but also by the external action of a local quantum observer that controls the coherence of the device. Depending on how and where the observation takes place the direction of heat and particle currents can be independently controlled. In fact, we show that the current and heat flow can go against the natural temperature and voltage gradients. Dynamical quantum measurement offers new possibilities for the control of quantum transport far beyond classical thermal reservoirs. Through the concept of local projections, we illustrate how we can create and directionality control the injection of currents (electronic and heat) in nanodevices. This scheme provides novel strategies to construct quantum devices with application in thermoelectrics, spintronic injection, phononics, and sensing among others. In particular, highly efficient and selective spin injection might be achieved by local spin projection techniques.

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Classical non-equilibrium thermodynamics was developed to understand the flow of particles and energy between multiple heat and particle reservoirs¹. The best-known example is Clausius' formulation of the second law of thermodynamics stating that heat cannot flow from a cold bath to a hot one². This is firmly based on the assumption that a macroscopic body in equilibrium is characterized by a single parameter: its temperature. When two objects with different temperatures are brought in contact, heat will flow from the hotter to the colder one. In macroscopic objects, the observation of this process does not influence the flow of energy and particle between them. However, when moving towards the nanoscale, quantum effects have to be considered and some thermodynamical concepts have to be revisited^{3,4}. In this quantum world, states of matter can be set into a coherent superposition, such as the famous Schrödinger's cat. When a macroscopic observer measures a nanoscale system, this interaction destroys most of the coherence inside the system and alters its dynamical response.

However, if a quantum observer instead acts only locally, the system quantum coherence changes continuously and dynamically. Depending on how strong and where these local quantum measurements are performed, novel and surprising quantum transport phenomena might arise. Decoherence⁵, for instance, has been shown to affect the dynamical evolution and decoupling from the environment via the Quantum Zeno effect^{6,7}, the rate of cooling⁸ and the efficiency of energy transport in molecular devices^{9,10} and biological systems^{11,12,13}. Here, to include the role of the quantum observer into a complete consistent thermodynamic formalism, we will use an external quantum bath that changes quantum coherences in the basis defined by the observer. In contrast to standard reservoirs in classical thermodynamics, described to be in an ensemble thermal state, our quantum coherent bath has no temperature parameter that can be associated to it¹⁴. This offers further possibilities for the control of quantum transport far beyond classical reservoirs. The present work focuses on the role of this particular quantum observer and the non-equilibrium thermodynamic^{15,16,17} implications it has on both particle and energy transport through thermo-electric nanodevices. Surprisingly, we find that the quantum observer can independently control heat and particle current, both in direction and strength. Therefore, incorporation of the concept of a quantum observer can lead to novel strategies to construct quantum devices with application in thermoelectrics, spintronic injection, phononics, and sensing, to just name a few. For instance, controlling the direction and strength of the heat flow will improve the figure of merit of thermoelectric devices by decreasing the thermal conductivity and outperform current technologies. In addition, the projection of only one component of the spin might open the path towards an efficient polarized spin injection strategy.

Results

To illustrate the new phenomena induced by the quantum observer, we consider the general and standard transport device shown in Fig. 1. Without loss of generality, this device is modeled by a simple tight-binding Hamiltonian with uniform on-site energy ϵ_0 of 1eV and nearest-neighbor hopping of 0.5 eV. For simplicity, we assume a single electron to be present in the device, though the results would not change if many electrons were active. This configuration can easily be realized experimentally in silicon heterostructures¹⁸, with cold atoms¹⁹ or in graphene²⁰. Our findings are universal and apply to more general nanodevices: The geometry of the device modifies the absolute value of the current flows but not the effect itself. The nine leftmost and rightmost sites are connected to macroscopic thermal baths at different temperature. As a result energy and particles will flow equally through the two branches. For the sake of simplicity in all this work we set the external voltage gradient between the reservoirs to zero; all effects in heat and particle flows come from the thermal gradient and the quantum observer alone. Adding an external bias voltage would introduce another source of current but would not modify the

conclusions concerning the impact of the quantum observer in the dynamics of the energy and particle flow in the nanodevice. While in this configuration energy can be exchanged via the baths, particle current is then corralled inside the device. At steady state no particle current is present, however, constant heat flows from hot to cold according to the second law of thermodynamics.

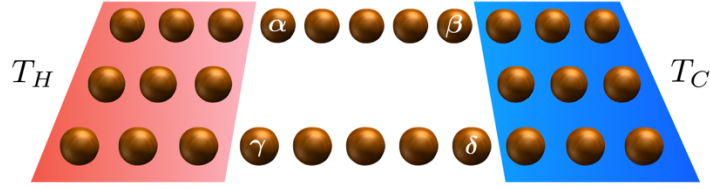


Figure 1 | Sketch of the thermo-electric transport nanodevice studied here. The nine leftmost and rightmost atoms are connected to thermal baths at temperature T_H and T_C , respectively. Due to this temperature imbalance heat flows from the hot to the cold side equally through the two identical branches. This device will be used to study physical phenomena arising from local quantum observations. We tested similar devices with different geometries and lengths of the two branches. The conclusions drawn with the present configuration remain valid.

While the coupling to the two thermal baths is modeled by a standard master equation²¹, the quantum observer acts on one site changing the quantum coherence only as in the double-slit experiment²². The quantum observer is assumed to be in a pure quantum state rather than in an ensemble temperature-state as the thermal baths are. We are interested here in understanding how the particle and heat currents change when the quantum observation acts on a specific site, as indicated by the eye in Fig. 2a. For that specific case, Fig. 2b shows the heat current through the device as a function of the coupling strength to the quantum observer γ_D and the amplitude of the applied thermal gradient ΔT . A positive current (red) indicates a flow from left to right. While the upper curved surface shows the energy current in the upper branch of the device, j_{up}^h , the flat contour-plot below corresponds to the energy flow in the lower branch, j_{down}^h . We emphasize that this contour plot is a projection onto the plane, hence only the color gradient indicates its strength. When the quantum observer measures the system at site labeled α , the energy current increase in the natural direction of the thermal gradient. However, even in the absence of a thermal gradient, the effect of the observation is to create a quantum heat flow from left to right. Remarkable, this local observation induces also a particle current in the upper branch from left to right, as can be clearly seen in Fig. 2c. As this situation corresponds to a steady-state, the corresponding particle current in the lower branch is exactly the opposite of it. As a result of the local action of the observer at site α , an unexpected particle ring-current is induced in the device that flows in clockwise direction. By symmetry, a similar measurement on site γ would give a counter-clockwise ring-current.

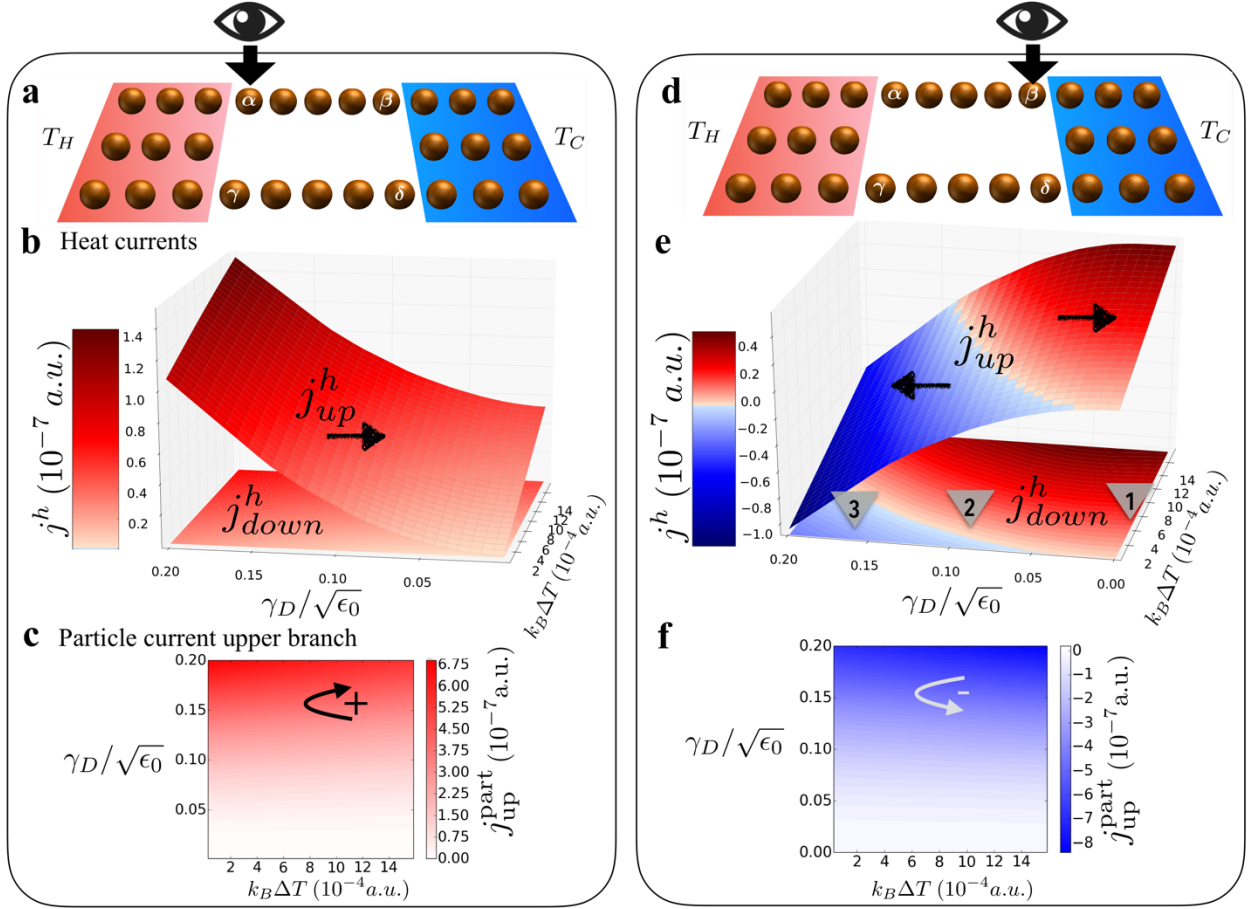


Figure 2 | Particle and energy currents in the steady state. In **a–c** the observation is performed at site α , while in **d–f** on site β . **b** and **e** show the heat current in the upper, j_{up}^h , and lower branch, j_{down}^h . A positive current (red) indicates heat flowing from left to the right. While the upper current is plotted as a curved surface, the lower energy current has been projected onto a plane to allow comparison of both. In **c** and **f** the particle current in the upper branch is shown. A positive current indicates that a particle ring-current is flowing clockwise. The triangles labeled 1, 2 and 3 in **e** mark regions where the energy flow is to the right in both branches, in different directions in each branch, and to the left in both branches, respectively. A temperature gradient of 10^{-3} a.u. corresponds to around 300 K, and a particle current of 3×10^{-7} a.u. corresponds to 2 nA.

We now consider how this situation is modified when we change the observation site from α to β , indicated in Fig. 2d. Most surprisingly, now the heat flows change direction as seen in Fig. 2e: When no observation is performed (triangle 1), heat goes from the hot to the cold reservoirs in the upper and lower branches as expected. However, beyond a certain observer coupling strength γ_D (triangle 3), the *energy moves in both branches against the thermal gradient*, that is, heat goes from the cold to the hot bath. Additionally, for intermediate coupling strength γ_D (triangle 2) we observe energy ring-currents in counter-clockwise direction. Interestingly, the observation induces now a *counter-clockwise* particle ring-current, as can be seen in Fig. 2f. This is a consequence of the localization of the electronic state induced by the local observation. As the electronic density in our model is just four times larger in the leads than in the branches, the quantum observer acting on site β pulls the electron out of the right lead pushing it towards the left lead. An electronic current starts to flow in the upper branch from right to left. When instead the observation is performed close to the left lead, the particle flows in the opposite direction.

Having heat flowing from a cold bath to a hotter one may appear as an apparent violation of Clausius' formulation of the second law of thermodynamics. In order to understand that this is not the case, we examine the situation in terms of basic non-equilibrium thermodynamic entropy concepts². The general entropy production rate equation²³ can be written as

$$\dot{S} = \Phi + P, \quad (1)$$

where S is the total entropy of the system, Φ is the net entropy flow into the system and P is the entropy production due to irreversibility inside the system that is always positive. For a system in the steady state between two temperatures, T_H and T_C , \dot{S} should be zero and

$$\Phi = \Phi_H + \Phi_C = -\frac{\dot{Q}_H}{T_H} - \frac{\dot{Q}_C}{T_C} = -P. \quad (2)$$

Here, \dot{Q}_H and \dot{Q}_C denote the heat flows to the hot and cold reservoirs, respectively. This leads to the following equation

$$\frac{\dot{Q}_H}{T_H} + \frac{\dot{Q}_C}{T_C} = P \geq 0. \quad (3)$$

In the case that the only energy exchange happens via the two baths, the continuity equation, $-\dot{Q}_H = \dot{Q}_C$, leads to the familiar concept that heat goes from hot to cold reservoirs. However, by introducing the coupling to the quantum observer, it is indeed possible to have heat flowing in more complicated ways, even against the thermal gradient. This is because the observer can create an energy flow even if it does not have a temperature associated to it. The new energy source changes the continuity equation to $\dot{Q}_H + \dot{Q}_C + \dot{Q}_D = 0$, where \dot{Q}_D is a purely quantum coherent heat flow introduced by the observation process. This quantum bath does not add a new entropy flow to Eq. (2) (as shown in Methods), but changes the particle and heat flows. The observer effectively acts as a quantum source of heat by changing the entropy production P directly and breaking the symmetry of the system. This creates changes in the steady state in analogy to dissipative structures²³. Classical dissipative structures have been used to explain non-equilibrium systems such as living organisms or hurricanes²⁴. Like in classical dissipative structures the increase in entropy production, due to the quantum measurement, leads to the observed reversal of entropy flows in our device (See SI).

To show that this new effect is general and gives rise to even more interesting applications and quantum phenomena in more complex nanoscale systems, we next consider another device similar to the famous 'Feynman's ratchet'²⁵. Quantum ratchets are transport devices driven by thermal or quantum fluctuations that have been widely studied to control the flow of particles and heat^{26,27}. In order to model such a ratchet, we introduce the spatial asymmetry by changing the on-site energy levels on the parallel branches of our device shown in Fig. 3a. In the upper branch (sites $\alpha - \beta$), the on-site energies are increased steadily by 10% as we move from left to right, which is graphically indicated by the size of the spheres. In the lower branch instead, the on-site energies increase from right to left in equal proportion. Therefore, we have created a quantum ratchet by adding two rectifiers on each branch in opposite direction. This could be experimentally realizable with techniques developed for constructing quantum ratchets in graphene²⁰, atom traps²⁸ or for molecular junctions²⁹. This configuration is chosen here to illustrate the differences of making a quantum observation in the top or bottom branches by breaking the top-down symmetry of the original device of Fig. 1. First, Fig. 3c shows that even without an observation a particle current flows in clockwise direction. This is because the system acts similar as a "salmon ladder" for our chosen working temperature³. In the upper branch for instance, there is a small probability of the particle to hop from the left side each step up the

ladder due to thermal fluctuations, but there is a very low probability for the particle on the right side to climb up the big drop of the ladder to then go down the ladder. Most interestingly, by adding a quantum observation on site β , the particle current decreases and later goes against the natural direction of the ratchet. This effect can be explained by similar arguments as before for the flat geometry. We highlight that the particle current changes its direction under very weak coupling to the quantum observer. This device could hence be used for sensing applications with nanoscale resolution observing weak quantum effects. The energy currents, as illustrated in Fig. 3b, have similar regimes as discussed before. When the observation is instead performed at site δ , in the bottom branch, the particle current is always in the preferred direction of the ratchet, but it can be significantly increased with stronger observation strength (See Supplemental Material).

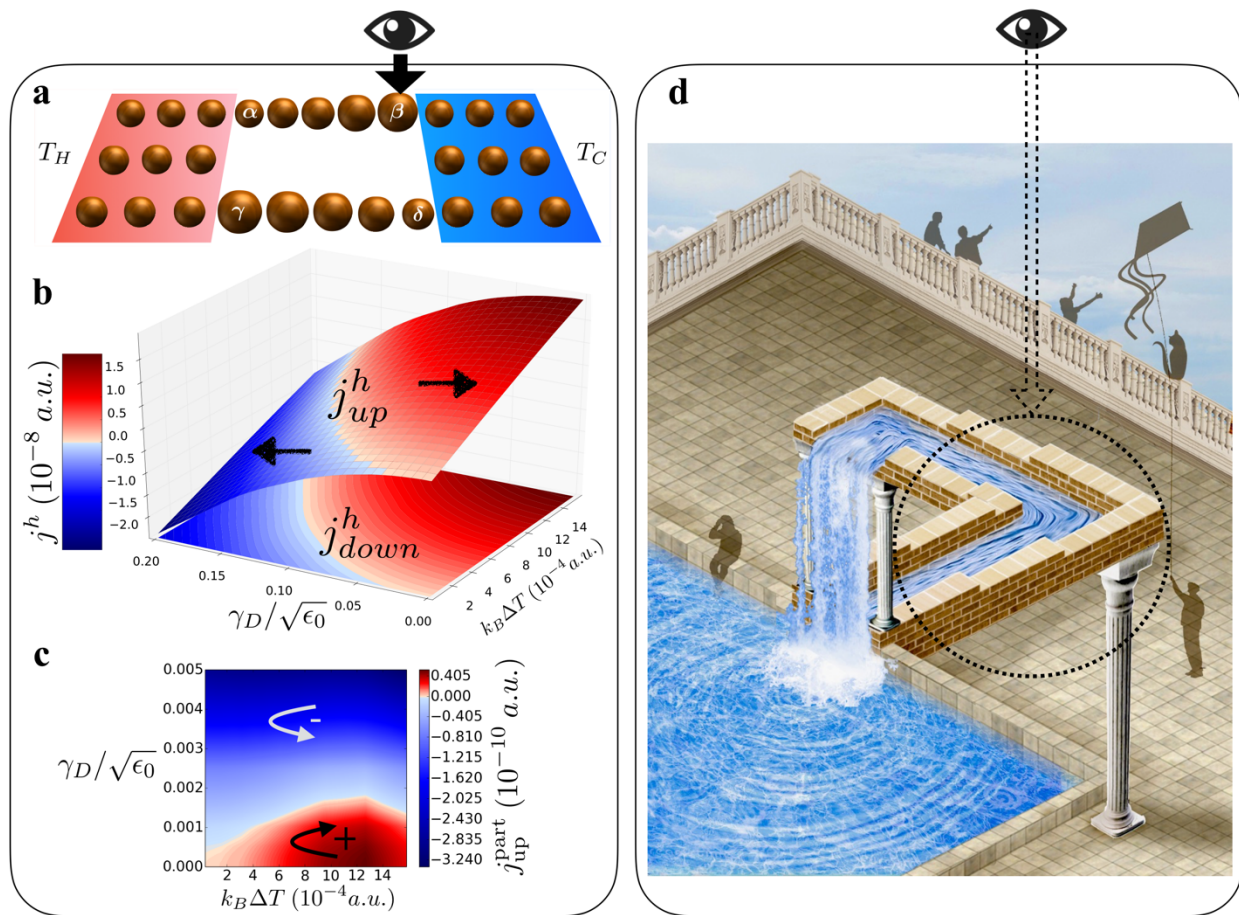


Figure 3 | Influence of a quantum observation on the thermo-electric flows in a quantum ratchet.

(b) Change of the energy currents in the top (j_{up}^h) and bottom (j_{down}^h) branches due to the influence of a local measurement on site β . (c) The particle current in the upper branch can be seen. It is striking in c that the particle ring-current can change direction as a function both of γ_D and ΔT . (d) Artistic illustration of the role of a quantum observer in a nanodevice: When observing inside the black circle, it appears the water flows down the channel, instead, by looking at the whole painting the water actually flows uphill. This apparent paradox mimics the coherent superposition of two quantum states (water flowing up/down). By observing at specific parts of our system we are able to tune between these two states and hence change the ‘physical response of the nanodevice’ in a controlled way.

In conclusion the results presented here indicate that particle and energy currents can be created and controlled by the mere presence of a quantum observer. This at first glance surprising behavior can be illustrated with an Escher-like drawing shown and explained in Fig. 3d. The present work can be further connected to the concept of entropy-driven organized dynamical systems, also known as dissipative structures²³. However, in our nanodevice, the increase in entropy production comes from a purely quantum mechanical source. We have shown that understanding and controlling the role of a quantum observer can lead to advances in thermoelectric devices. Additionally, a quantum observer can be used for novel ways of creating and controlling energy and particle transport that can have applications for spintronic injection, quantum phononics, and sensing. For example a local observer can act as a magnetic memory writer that projects out one of the spin components, giving raise to a complete spin-polarized current even in the absence of spin-orbit coupling. It also highlights the role of an observer in quantum devices: While in the famous Schrödinger's cat paradox the coherent state is destroyed directly via the observation by a classical object, here we have shown that a local quantum observer changes coherence locally and dynamically modifying the heat and electronic transport behavior of the device. Quantum measurements offer new possibilities of thermodynamic control for quantum transport³⁰ far beyond classical thermal reservoirs.

Methods

Our device in Fig.1 is modeled by the simple one-electron Hamiltonian

$$H = \sum_i \epsilon_i c_i^\dagger c_i - \mathcal{T} \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i), \quad (4)$$

where $\langle i, j \rangle$ is the nearest neighbor index and c_i^\dagger creates an electron at site i . For simplicity, only one electron is present in our study. To introduce a thermal imbalance ΔT in the transport device, we connect the nine leftmost and rightmost atoms to thermal baths kept at temperature T_H and T_C respectively. These temperatures are chosen around an average temperature T_E such that $T_{H,C} = T_E \pm \Delta T$. The state of the system evolves according to a standard Markovian master equation²¹ (All equations are written in atomic units):

$$\begin{aligned} \frac{d\rho}{dt} &= -i[H, \rho] + \sum_{\alpha=H,C,D} (K_\alpha \rho S_\alpha + S_\alpha \rho K_\alpha - S_\alpha K_\alpha \rho - \rho K_\alpha S_\alpha) \\ &= -i[H, \rho] + \sum_{\alpha=H,C,D} \mathbb{L}_\alpha[\rho], \end{aligned} \quad (5)$$

where $K_{H,C} = \lambda^2 \int_{-\infty}^{\infty} C_{H,C}(\tau) e^{-iH\tau} S_{H,C} e^{iH\tau} d\tau$ describes the influence of the two thermal baths onto the system. We point out that the master equation (5) has the same steady-state solution as a second-order non-Markovian master equation²¹. The bath-correlation function C for the hot and cold thermal baths can be derived from first principle by assuming the electronic system is in contact with the radiation inside a cavity^{21,31}

$$C_{H,C}(\tau) = \frac{1}{2\epsilon_0\pi} \int_0^{\omega_c} d\omega \{ [n_B(\omega, T_{H,C}) + 1] e^{-i\omega\tau} + n_B(\omega, T_{H,C}) e^{i\omega\tau} \}, \quad (6)$$

where n_B is the Bose-Einstein distributing function and ω_c a cut-off frequency due to the dipole approximation. Furthermore, the coupling operator S in Eq. (5) is given by

$$S_{H,C} = -\mathbf{u} \cdot \mathbf{r} M_{H,C}(\mathbf{r}), \quad (7)$$

where e is the electron charge, \mathbf{u} the polarization direction of the modes in the cavity (all three spatial coordinates) and $M_{H,C}(\mathbf{r})$ is a mask function that is either one for \mathbf{r} in the hot and cold region or otherwise zero. This will model the local coupling at the left or right ends of the device. This choice of the bath-correlation function (6) and the coupling operators (7) can be derived from first-principles³¹ and ensures that the system relaxes towards thermal equilibrium in the case of zero temperature gradient ($T_H = T_C$). This is indeed the case in our simulations. In order to account for the local quantum measurement within the same thermodynamic formalism, we consider

$$K_D = \frac{\gamma_D^2}{2} |k\rangle\langle k| \quad (8)$$

and $S_D = |k\rangle\langle k|$, where k indicates the site where the observer is acting with observation strength γ_D . In this way, the quantum observer changes quantum coherences to site k continuously and dynamically. This kind of measurement does not freeze the dynamics, like in the quantum Zeno Effect, but does affect the final steady state and thus the macroscopic measurable thermodynamic flows. This effect of local observation can come from a quantum observer of the kind discussed in [8] or for example from electron-phonon coupling.

In order to study the energy flows through our transport device, we define the local energy-density operator $h_i = -\frac{1}{2}\mathcal{T}\sum_{\langle j\rangle}(c_i^\dagger c_j + c_j^\dagger c_i) + \epsilon_i c_i^\dagger c_i$ where the summation is over the neighboring sites. Then, the continuity equation, $-\frac{dh_i}{dt} = -i[H, h_i]$, is used to define the energy-current operator³² that describes the heat flow in the middle of the upper branch, j_{up}^h , and lower branch, j_{down}^h . Moreover, by considering the electronic density the particle current j_{up}^p in the upper branch is defined in a similar way.

As parameters for the model, we chose $\epsilon_0 = 1 \text{ eV} = 0.036 \text{ a.u.}$, $T = \epsilon_0/2$, $\lambda/\sqrt{\epsilon_0} = 0.2$ and $k_B T_E = 0.008 \text{ a.u.}$ We studied further ranges of T_E but we will present this in a future publication. We considered devices in two configurations. In the flat configuration, as seen in Fig. 1, all sites have the same on-site energy ϵ_0 . The second configuration studied is the quantum ratchet seen in Fig. 3a. For that, the sites of the right and left leads have energy ϵ_0 . Sites α to β form a ladder of equal steps in energy of 0.1 eV, such that $\epsilon_\alpha = 1.1 \text{ eV}, \dots, \epsilon_\beta = 1.5 \text{ eV}$. Sites γ to δ form a ladder of equal steps of 0.1 eV in the opposite direction, such that $\epsilon_\gamma = 1.5 \text{ eV}$ and $\epsilon_\delta = 1.1 \text{ eV}$. Because these rectifiers are anti-parallel, they create a preferred clockwise particle flow as explained in the main text.

A quantum observer has zero entropy flow. Examining the entropy flow due to the local observation shows that the quantum observer does not add a new entropy flow to the system in contrast to a standard thermodynamic heat bath. For the coupling described by the master equation (5), the entropy flow into the system due to the local observer can be written as¹⁴

$$\Phi_D = -\text{Tr}[\mathbb{L}_D[\rho] \ln \sigma_D]. \quad (9)$$

Here, σ_D is the stationary state of the local quantum observation at site k , $\sigma_D = |k\rangle\langle k|$, and \mathbb{L}_D is defined in Eq. (5) and leads to

$$\mathbb{L}_D[\rho] = \gamma_D^2 [2 |k\rangle\langle k| \rho |k\rangle\langle k| - |k\rangle\langle k| \rho - \rho |k\rangle\langle k|]. \quad (10)$$

Inserting this equation into Eq. (9) shows that the entropy flux due to the quantum observer is zero. This means that a quantum observer changes the energy flow in the system directly, without having an entropy flow connected with it.

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Author contributions

All authors have contributed significantly to this work. R.B. and C.A.R.R. provided theoretical support and performed the simulation and data analysis. A.R. and T.F. conceived, designed and led the research.

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Supplemental Material

Quantum ratchet locally measured at site δ .

For completeness we show the results when the quantum observer acts at site δ for the quantum ratchet. Without the action of a local observer the particle current flows in counter-clockwise direction. This steady-state current can be increased in this direction by the action of the quantum observer at site δ , as shown in Fig. S1b. Additionally, the local quantum observation can control the energy current as shown in c.

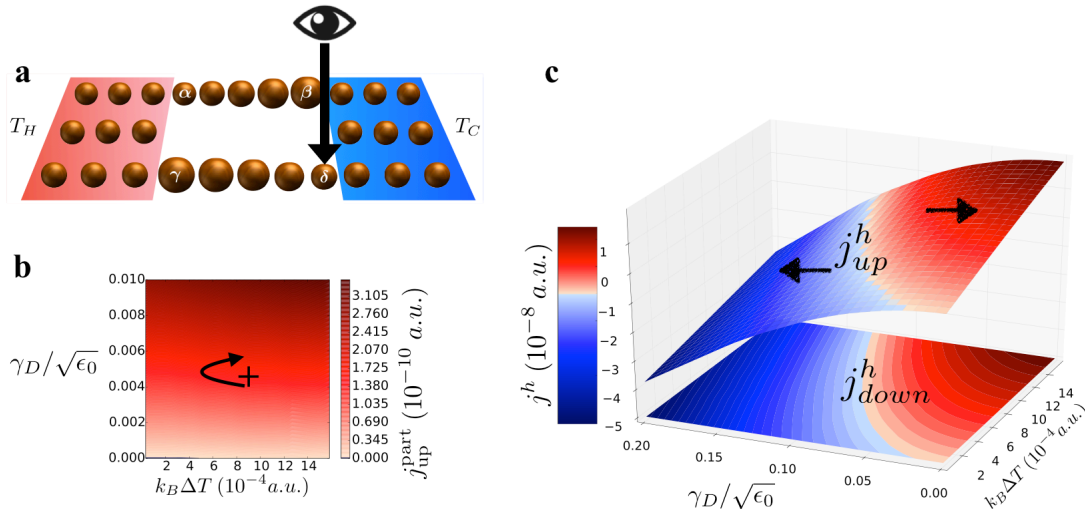


Figure S1 | Influence of a quantum observation at site δ on the thermo-electric flows in a quantum ratchet. Plot c shows the different energy currents in the top (j_{up}^h) and bottom (j_{down}^h) branches while b shows the particle current in the upper branch, all as a function of the coupling to the quantum observer (γ_D) and temperature difference ($k_B\Delta T$).

Small changes in entropy production lead to reversal of entropy flow.

Figure 5 illustrates that small changes in the entropy production rate (a) introduced by the coupling to the quantum observers leads to a change in the direction of thermodynamic flows (b). The difference between the changes of entropy production and entropy flow as a function of the measurement strength drives the regimes of transport. Quantum measurements can change the steady-state dynamics in ways analogous to dissipative structures [23]. Dissipative structures are dynamical states of matter that depend strongly and in complicated ways to the amount of entropy production. In our model, the local action of the quantum observer also adds irreversibility that breaks the existing symmetries of the device, in turn, changing the direction of the heat flow and creates particle ring-currents.

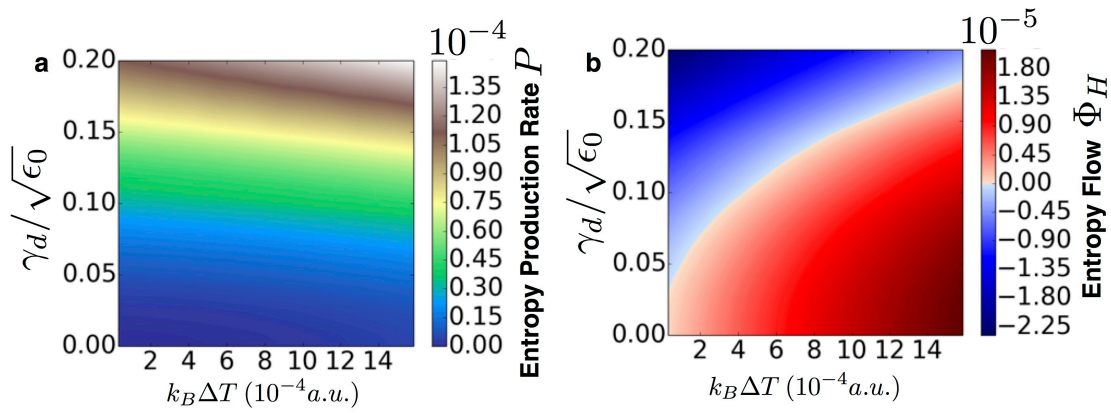


Figure S2 | Entropy Production Rate and Entropy Flow to the hot bath for the ratchet device in Fig. 3a. These quantities are defined in Eq. (2) in the main text. (a) The entropy production rate increases with increasing temperature gradient ΔT and increasing observer coupling. (b) Under the same conditions the entropy flow from the hot bath changes differently in comparison to the entropy production rate, even changing signs. This illustrates how minor changes in the entropy production rate can lead to abrupt changes in the thermodynamics flows.