Non-equilibrium quantum many-body Rydberg atom engine

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The standard approach to quantum engines is based on equilibrium systems and on thermodynamic transformations between Gibbs states. However, non-equilibrium quantum systems offer enhanced experimental flexibility in the control of their parameters and, if used as engines, a more direct interpretation of the type of work they deliver. Here we introduce an out-of-equilibrium quantum engine inspired by recent experiments with cold atoms. Our system is connected to a single environment and produces mechanical work from many-body interparticle interactions arising between atoms in highly excited Rydberg states. As such, it is not a heat engine but an isothermal one. We perform many-body simulations to show that this system can produce work. The setup we introduce and investigate represents a promising platform for devising new types of microscopic machines and for exploring quantum effects in thermodynamic processes.

Engines are devices able to convert some form of energy into mechanical work. The most famous examples, heat engines, operate by exchanging heat with (at least) two thermal reservoirs at different temperatures [1–4]; other working principles can be implemented also with a single reservoir [5–7]. Nowadays, due to significant technological breakthroughs in manipulating and controlling microscopic systems, a new focus is on devising and realising efficient machines harnessing quantum effects [7–12]. To explore possible avenues at this scale, quantum thermodynamics has been put forward as a theoretical framework merging features of quantum physics with the laws of thermodynamics [13–15]. While much progress has been made in theoretically describing quantum engines, it is often not clear how energy, in the form of mechanical work, can be extracted from a many-body quantum system.

Here, we present and analyse a quantum engine whose working system is described by genuine non-equilibrium many-body steady-states and not by thermal states (see, e.g., [16, 17]), as is more standard. This novel feature comes at an additional cost in terms of efficiency: maintaining a non-equilibrium steady-state requires the constant injection of energy which is continuously dissipated. Current experiments allow for the implementation of such driving protocol and for the precise control over the emerging non-equilibrium states. We present our ideas in the context laser driven Rydberg atoms [see Fig. 1(a)] arranged in a one-dimensional (1D) chain, e.g. achieved by means of optical lattices or optical tweezer arrays [18–28]. In this scenario, we envisage for the sake of illustration a movable "piston" subject to the (repulsive) force between Rydberg excited atoms and allowing one to tune the volume of the chain, as shown in Fig. 1. In current setups, the length of the chain is not a dynamical degree of freedom but rather a parameter that can be externally controlled. As we show in this article, this setting is already sufficient to experimentally determine the amount of work that can be generated with our engine.

This physical setup offers a transparent interpretation of the engine, sketched in Fig. 1(b), in particular in terms of the nature of the work it can provide. The laser pumps energy (input) into the system which converts it into interaction energy of Rydberg states, and which can then be extracted through the mechanical motion of the piston (output). The system thus acts as an opto-mechanical energy converter, with spontaneous decay of Rydberg excited states leading to constant energy losses during the cycle. The periodic protocol we consider consists of two isochoric transformations, which increase or decrease the density-density interactions of the Rydberg "working fluid", and of two transformations where the volume is varied. This cycle is illustrated in Fig. 1(c) through an analogy with a classical engine.

Going beyond previous proposals, our engine is based on a genuine non-equilibrium protocol, which we investigate from a fully dynamical, i.e. explicitly time-dependent, viewpoint [16, 17]. Unlike recent work, see e.g. Refs. [16, 29, 30], we provide nonperturbative results for open many-body quantum systems beyond the mean-field approximation. Moreover, our device is not a heat engine but rather an isothermal engine [6] operating far from equilibrium in contact with a single environment. From an experimental viewpoint this approach provides a substantial simplification since the engine does not need to alternate between two different heat baths [17]. Our setup can be used to design realistic quantum devices or as a new testbed to explore the impact of quantum effects on thermodynamic processes

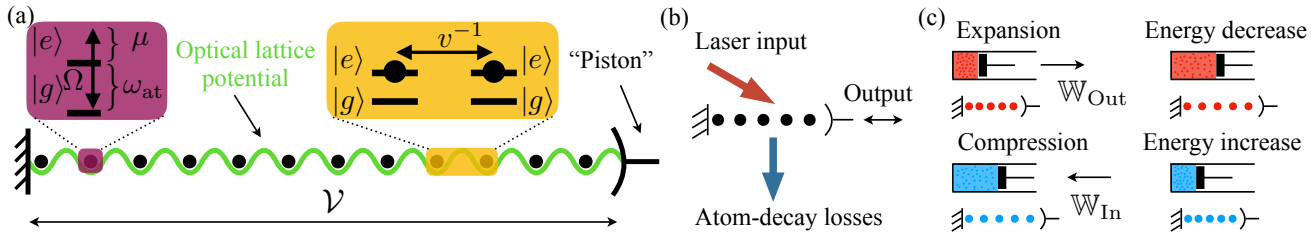

FIG. 1. **Rydberg atomic chain and schematics of the engine.** (a) Array of Rydberg atoms confined in a 1D geometry. Each atom is modeled as a two-level system with ground state $|g\rangle$, excited (Rydberg) state $|e\rangle$ and level splitting $\omega_{\rm at}$. Laser driving generates oscillations, $|g\rangle \leftrightarrow |e\rangle$, at Rabi frequency Ω; transitions can be made off-resonant through the detuning μ. The volume $\mathcal{V}$ can be tuned through a movable "piston" or mirror. This control mechanism changes the interatomic distance thus modifying the interaction strength , v^{-1}, between neighboring excited atoms. (b) Sketch of the Rydberg atom engine. The quantum system is driven out-of-equilibrium by a laser injecting energy which can be lost through atom decay. By means of an appropriate periodic manipulation of the "piston", the system can deliver positive net output work. (c) Four-stroke cycle and analogy with Rydberg atomic engine. During the expansion work $\mathbb{W}_{\rm Out}$ is extracted. This stroke is followed by a *cooling* step decreasing the interaction energy of the working fluid. Then a compression performs work $\mathbb{W}_{\rm In}$ on the system, and a *heating* step increases the interaction energy. Cooling and heating are implemented by varying the laser detuning.

far from equilibrium. Finally, our framework provides, at least in principle, a viable mechanism for direct work measurement and extraction; the piston is a macroscopic object, whose position couples to the interaction energy of the atoms, and all relevant quantities that characterise our engine are accessible experimentally by measuring density correlation functions through spatially resolved imaging of Rydberg excitations [31].

The model– We consider a 1D array of laser driven Rydberg atoms. The Hamiltonian, in a frame rotating with the laser frequency, is given by [32] [*c.f.* Fig. 1(a)]

$$H = \Omega \sum_{k=1}^{N_{\rm at}} \sigma_x^{(k)} - \mu \sum_{k=1}^{N_{\rm at}} n^{(k)} + H_{\rm LG}^{v} \,. \tag{1}$$

Here, $\sigma_x |g/e\rangle = |e/g\rangle$, while n counts the presence of an excitation $n|e\rangle = |e\rangle$ and $n|g\rangle = 0$. $N_{\rm at}$ is the total number of atoms. The first two terms are related to the laser driving. The term $H_{\rm LG}^{v}$ is the *lattice gas* Hamiltonian accounting for classical (i.e. diagonal) volume-dependent (repulsive) nearest-neighbour interactions,

$$H_{\rm LG}^{v} = \frac{1}{v} \sum_{k=1}^{N_{\rm at}-1} n^{(k)} n^{(k+1)} \,.$$

This operator represents the mechanical energy that is stored in the system and can be altered by changing the inverse interaction strength v through variations of the volume of the 1D array of atoms, see Fig. 1(b-c).

The roles played by the other terms in the Hamiltonian (1) are as follows: the one proportional to Ω leads to excitations being created and annihilated. This parameter is not altered during the cycle; it rather provides the system with the background fluctuations needed to generate atomic transitions between $|g\rangle$ and $|e\rangle$. Transitions are further controlled by the detuning term μ. Large detunings make transitions off-resonant, suppressing the probability amplitude of observing excitations or de-excitations. Combining this observation with the fact that the system also experiences spontaneous atomic decays [see Eq. (2) below], one would expect to observe, on average and after a transient, a larger number of Rydberg excitations for small detunings μ. Indeed, when the detuning is large, atoms which are found in the ground state after decaying are less likely excited due to the transition being off-resonant. This effect leads to a lower Rydberg state population and, in turn, to a lower interaction energy. Hence, varying the parameter μ makes it possible to modify the interaction energy of the Rydberg system without changing its volume; this allows us to realise the engine cycle as discussed in Fig. 1(c).

In order to account for the spontaneous decay of excited states, which is indeed a non-negligible feature of experiments, we exploit a Markovian dissipative map in Lindblad form [33, 34]. The latter is defined for atom decay as

$$\mathcal{L}[X] := \gamma \sum_{k=1}^{N_{\rm at}} \left(\sigma_-^{(k)} X \sigma_+^{(k)} - \frac{1}{2} \left\{ n^{(k)}, X \right\} \right) . \tag{2}$$

Here, γ^{-1} represents the characteristic life-time of the Rydberg state, and $\sigma_- |e\rangle = |g\rangle$, $\sigma_+ = \sigma_-^\dagger$. Altogether, the system density matrix ρ_t evolves, in the rotating frame, through the equation

$$\dot{\rho}_t = -i[H, \rho_t] + \mathcal{L}[\rho_t] \,. \tag{3}$$

This model for laser driven Rydberg systems is, in fact, phenomenological. Still, it is commonly used to interpret cold-atom experiments as it enables a quantitative description of atomic interactions and has been extensively tested in practice. Note that the dissipative generator of Eq.(2) contains local Lindblad operators even though the Hamiltonian H involves interactions. This feature

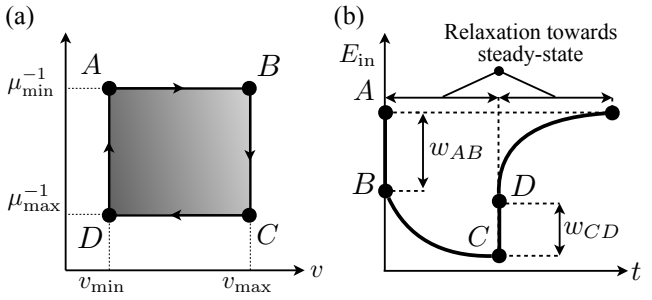

FIG. 2. **Periodic driving and representative cycle of the internal energy.** (a) Periodic driving protocol in the Rydberg system. The parameters in the various transformation are varied through sudden quenches. (b) Representative instance of the time-dependent internal energy for the cycle shown in (a). Sudden jumps in $E_{\rm in}$ are associated with work exchanges through the interparticle interactions (negative in the expansion). Curves with finite derivative represent relaxation after quenches in the laser detuning parameter μ.

can lead to violations of the second law in generic instances [35–39]. However, as we show below, in our *zero-temperature* setup, in which only atom decay plays a role [37], there are no thermodynamic inconsistencies.

Internal energy, first law and engine cycle– In order to discuss the engine depicted in Fig. 1 and the net output that it can deliver, we need to develop a thermodynamic description of the system. To this end, we first have to identify the *internal energy* of the engine, which corresponds to the energetic content in the working fluid that could, in principle, be extracted in the form of work. In our setup, this quantity is related to the repulsive interaction energy $H_{\rm LG}^v$ and to the single-atom energy

$$H_{\rm at} = \omega_{\rm at} \sum_{k=1}^{N_{\rm at}} n^{(k)} \,,$$

associated with the energy difference, $\omega_{\rm at}$, between excited and ground state, see Fig. 1(a). We thus define the system energy operator, $H_{\rm in}^v$, as

$$H_{\rm in}^v := H_{\rm at} + H_{\rm LG}^v \tag{4}$$

and the specific internal energy as

$$E_{\rm in}(t) := \frac{1}{N_{\rm at}} \operatorname{Tr}\left[\rho_t \, H_{\rm in}^v\right]\big|_{v=v_t} . \tag{5}$$

The contribution $H_{\rm at}$ does not appear in Eq. (1) since the latter represents the Hamiltonian of the system in the interaction picture. The thermodynamic balance however must be formulated in the Schrödinger picture [40]. The unitary connecting Schrödinger and interaction picture has a generator proportional to $(\mu + \omega_{\rm at}) \sum_k n^{(k)}$, which commutes with $H_{\rm in}^v$. Therefore, after identifying the internal energy we can derive the thermodynamic balance using Eq. (3). The choice of the internal energy in Eq. (5) derives from a microscopic picture where the atomic chain, i.e., the system proper, is perturbed by the laser and the interaction with a thermal environment. In this setting, the Hamiltonian terms proportional to Ω and μ describe the interaction of the system with a laser, while the dissipative term, proportional to γ, describes its interaction with an environment. The actual internal energy of the atom system is thus solely associated with the Hamiltonian term in Eq. (4).

The first law thus reads

$$\dot{E}_{\rm in} = -f_t^{v_t}\, \dot{v}_t + I_t - J_t \,. \tag{6}$$

Here,

$$f_t^{v_t} = -\operatorname{Tr}\left[\rho_t \, \partial_v H_{\rm in}^v\right]\big|_{v=v_t} , \tag{7}$$

is the generalised force associated with the inverse interaction strength v, which is the only term in the internal energy responsible for mechanical work in our setup. The input power provided by the laser is given by

$$I_t = i \operatorname{Tr}\left[\rho_t \left[H_{\rm ex}^\mu, H_{\rm in}^v\right]\right]\big|_{v=v_t}^{\mu=\mu_t} ,$$

where the term $H_{\rm ex}^\mu = H - H_{\rm LG}^v$ corresponds to the laser-atom interaction. Finally, we have to account for the dissipated heat

$$J_t = -\operatorname{Tr}\left[\rho_t \, \mathcal{L}[H_{\rm in}^v]\right]\big|_{v=v_t} .$$

Note that, due to the form of $H_{\rm LG}^v$, this quantity is non-negative ($J_t \geq 0$) and vanishes only in the zero-excitation state. The environment is effectively at zero temperature as it is highly unlikely to observe spontaneous excitation of atoms at room temperature. Therefore, the above properties of J_t are sufficient to guarantee consistency with the second law: no heat is extracted from the zero-temperature environment.

The engine cycle we propose consists of a four-stroke periodic driving involving sudden quenches of the parameters μ and v, as depicted in Fig. 2(a). The presence of radiative decay is thereby of fundamental importance. This feature prevents the system from heating up to infinite temperature [41–43], as it would happen for an isolated engine. Instead, the system state approaches a non-trivial asymptotic cycle (see Supplemental Material [44]).

The actual cycle starts from A with a transformation given by a sudden expansion of the volume, resulting in a smaller interaction strength, $v_{\min} \to v_{\max} = v_{\min} + \Delta v$. During this expansion, work is extracted from the system. Afterwards, the system immediately undergoes a sudden quench $\mu_{\min} \to \mu_{\max} = \mu_{\min} + \Delta\mu$. In this transformation, no work is exchanged, but the system now evolves for a relaxation period, shown in Fig. 2(b), reaching a non-equilibrium state with a lower mean interparticle energy. The following sudden compression, reflected in $v_{\max} \to v_{\min}$, thus requires less work than is extracted

during the expansion. Immediately after the compression, the transformation $\mu_{\rm max} \to \mu_{\rm min}$ takes the system back to its initial state through a second relaxation period. In Fig. 2(b) we show a representative cycle of the internal energy following the periodic driving which further highlights the two relaxation periods in the cycle. In the regime depicted in Fig. 2(b), the engine delivers positive net output.

To quantify the net output of our Rydberg engine, we integrate the first law over a full period obtaining

$$w_{\rm net} := \int dt\, f_t^{v_t} \dot{v}_t = I - J\,,$$

where $I = \int dt\, I_t$ is the total input in one cycle and $J = \int dt\, J_t$ is the total dissipated heat. For $w_{\rm net} \geq 0$, we can thus define the efficiency of the engine as

$$\eta = \frac{w_{\rm net}}{I} = \frac{w_{\rm net}}{w_{\rm net} + J} \leq 1\,,$$

where the last equality follows from $J_t \geq 0$. Adapting these quantities to our driving protocol, we have

$$w_{\rm net} = -w_{AB} - w_{CD}$$

with (see [44])

$$w_{AB} = \left(\frac{1}{v_{\rm max}} - \frac{1}{v_{\rm min}}\right) \frac{1}{N_{\rm at}} \sum_{k=1}^{N_{\rm at}-1} \langle n^{(k)} n^{(k+1)} \rangle_A \leq 0\,,$$
$$w_{CD} = \left(\frac{1}{v_{\rm min}} - \frac{1}{v_{\rm max}}\right) \frac{1}{N_{\rm at}} \sum_{k=1}^{N_{\rm at}-1} \langle n^{(k)} n^{(k+1)} \rangle_C \geq 0\,. \tag{8}$$

In the above equations, $\langle\cdot\rangle_{A/C}$ is the expectation value taken over the non-equilibrium steady-state corresponding to the parameters in A/C, respectively. To produce net work, one needs to have $|w_{AB}| > |w_{CD}|$ [*cf.* Fig. 2(b)] which directly translates in $\sum_k \langle n^{(k)} n^{(k+1)} \rangle_A > \sum_k \langle n^{(k)} n^{(k+1)} \rangle_C$. Hence, interactions must be stronger during the expansion. Furthermore, as we are considering infinite relaxation periods, we have $J \to \infty$, since constant dissipation, also known as *housekeeping heat*, is required to maintain the non-equilibrium steady-state even if no thermodynamic transformation is performed. For finite relaxation times, where $J_t < \infty$, it is however possible to have a finite efficiency also in our non-equilibrium setting.

Simulation results– We now explore numerically the cycle as a function of the chosen values of $v_{\rm min}$ and $\mu_{\rm min}$. We fix $\Omega = \gamma = 1$ and assume that, after quenching μ, the system fully relaxes to its genuine quantum non-equilibrium steady-state.

In Fig. 3(a), we show the net work produced by an infinite system within a mean-field approximation. In Fig. 3(b), instead, we display numerically exact data

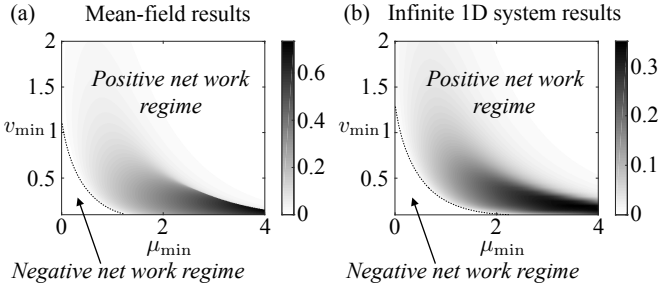

FIG. 3. **Dissipative infinite 1D Rydberg chain.** Phase diagram for a Rydberg engine. The parameters of the cycle for both plots are $\Omega = 1$, $\gamma = 1$, $\Delta v = \Delta\mu = 1$ and the relaxation time involved in the cycle is infinite. We focus on the stationary cycle. (a) Mean-field. The panel displays a density plot for the work delivered by the engine as a function of $v_{\rm min}$ and $\mu_{\rm min}$. It is indeed possible to have cycles that produce positive net work. (b) Infinite 1D Rydberg atomic system with nearest neighbour interactions. We observe the same qualitative features displayed by mean-field results. From a quantitative point of view, the work that can be extracted in an infinite 1D system differs from the one estimated in the mean-field approximation. In particular, the maximum amount of net work that can be extracted in a 1D system is smaller than predicted by the mean-field theory.

for a 1D chain obtained via infinite matrix product algorithms [50] (see [44] for details). First, we observe that it is indeed possible to extract net work from our cycle. Many-body simulations, accounting for quantum correlations in a nonperturbative way, confirm that this effect is not only a feature of the non-linear mean-field dynamics. In particular, a boundary arises in the phase diagrams of Fig. 3(a-b) separating a region where mechanical work can be extracted from the atomic array and a region where the system absorbs energy instead of delivering work. Additional finite-size and finite-relaxation results (see [44]) show unambiguously that positive output work can be extracted also in finite systems and very importantly also with finite relaxation times, i.e. with a finite efficiency.

Discussion– We have developed a many-body quantum engine that operates intrinsically under non-equilibrium conditions. While this design strategy, in contrast to conventional heat engine cycles, requires additional energy input to keep the working system in a non-equilibrium state (J_t does not vanish even at stationarity), it also allows for a more direct and efficient control of physical parameters, e.g. through external laser fields. Focussing on Rydberg atom ensembles, we have shown that it is possible to generate useful work.

In order to experimentally determine the amount of produced work, a measurement of density-density correlations is sufficient. In principle, it might even be possible to extract this work through a mechanical degree of freedom. In a hypothetical experiment, illustrated

in Fig. 1(a), this degree of freedom could be a movable mirror, which controls the spacing of the optical lattice trapping the atoms thus acting as a reciprocating piston. Assuming that it is possible to reach a parameter regime, where the interatomic separation is locked to the wavelength of the cavity mode, a direct coupling between the interaction energy and the mirror position can be established [44]. This mechanism would make it possible to transfer the output of our engine into a controllable work storage; its practical implementation therefore constitutes an important challenge for future experiments.

In our proposal, we did not consider the effect that measuring the position of atoms would have on the thermodynamic cycle and on fluctuations of the generated work. Instead, we have treated the position of the atoms as a classical parameter, in the spirit of a Born-Oppenheimer approximation. It would be interesting to derive from first principles a description of our engine which accounts for cross-correlations between position and momentum of the atoms and their electronic state.

It further remains an open question whether non-thermalising closed quantum systems, as in the case of many-body localisation [60–63] or prethermal metastable regimes due to almost conserved charges [64, 65], might be exploited to devise an isolated non-equilibrium many-body engine with a non-trivial cycle.

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