Quantum Szilard Engine with Attractively Interacting Bosons

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We show that a quantum Szilard engine containing many bosons with *attractive* interactions enhances the conversion between information and work. Using an *ab initio* approach to the full quantum-mechanical many-body problem, we find that the average work output increases significantly for a larger number of bosons. The highest overshoot occurs at a finite temperature, demonstrating how thermal and quantum effects conspire to enhance the conversion between information and work. The predicted effects occur over a broad range of interaction strengths and temperatures.

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The Szilard engine is an old thought experiment [1] that has become a paradigm for describing information-to-work conversion in thermodynamic systems. Originally, it consists of a single, classical particle confined in a hard-walled one-dimensional container of length L that can be divided by a moveable wall (i.e., a piston), and is coupled to a single heat bath. Using the information about the particle's location on either side of the piston, the engine transforms heat isothermally into work. The apparent contradiction to the second law of thermodynamics is resolved by accounting for the work cost associated with the information processing itself [2–8]: The erasure of one bit of information costs at least the entropy of $k_B \ln 2$. Only recently this was verified experimentally [9–12] for a single, *classical* particle. But yet, we know very little about how the fundamental relations [9,13–17] between work, heat, and information are altered by quantum effects and correlations [18–20] in interacting many-body systems.

In this Letter, we thus consider a number of N *interacting* quantum particles as the working medium. The Szilard cycle goes through the steps sketched in Fig. 1(a), carried out quasistatically and in thermodynamic equilibrium with a single surrounding heat bath at temperature T: (i) insertion of a wall at position ℓ^{ins}, (ii) measurement of the particle number n on the left side of the wall, (iii) reversible translation of the wall to its final position ℓ_n^{rem} that may vary from one cycle to another with different n, and (iv) removal of the barrier at ℓ_n^{rem}. In step (iii), the information about n allows extraction of work through the moving piston. In the classical limit, the insertion and removal of the wall can be achieved at no cost of work. In the quantum regime, however, this is no longer the case [21–24], since these processes shift the energy levels.

It is known that the average amount of work that in total can be extracted in a cycle crucially depends on the underlying quantum statistics. Without interactions, two bosons yield a higher work output than two fermions or classical particles [25]. Different facets of the quantum Szilard engine have been studied, including optimization of the cycle [26,27] or the effect of spin [28] and parity [29], but all for noninteracting particles. Interactions have so far only been discussed for two attractive bosons [30], where an increased work output was attributed to a classical effect.

An intriguing and yet unanswered question is, how the information-to-work conversion is affected by interactions. Classically, the performance of a Szilard engine with many noninteracting particles falls below that of the one- and two-particle engine—but, does this hold also for an interacting quantum gas?

Here, we demonstrate that attractive interactions indeed boost the information-to-work conversion in a bosonic Szilard engine. To that end we use a full quantum many-body treatment of spin-0 bosons with attractive interactions between the particles. We apply the two-body pseudopotential of contact type, $g\delta(x_1 - x_2)$, as commonly used for ultracold atomic gases [31]. The strength of the interaction g is given in units of $g_0 = \hbar^2/(Lm)$, where the energy unit is set by the single-particle ground state energy $\varepsilon_1 = \hbar^2\pi^2/(2mL^2)$ of the one-dimensional box considered here, and m is the mass of a single particle. A solution to the full quantum many-body problem can be obtained with very high numerical accuracy by exact numerical diagonalization (see Supplemental Material [32], which includes Ref. [33]). We find that a few-body system with attractive bosons generates an overshoot of work compared with $W_1 = k_B T \ln 2$. The maximum occurs at a finite temperature, illustrating the interplay between thermodynamic fluctuations and the many-particle excitation spectrum. Because the numerical cost of exact diagonalization becomes too large for $N > 4$, we also used an approximate,

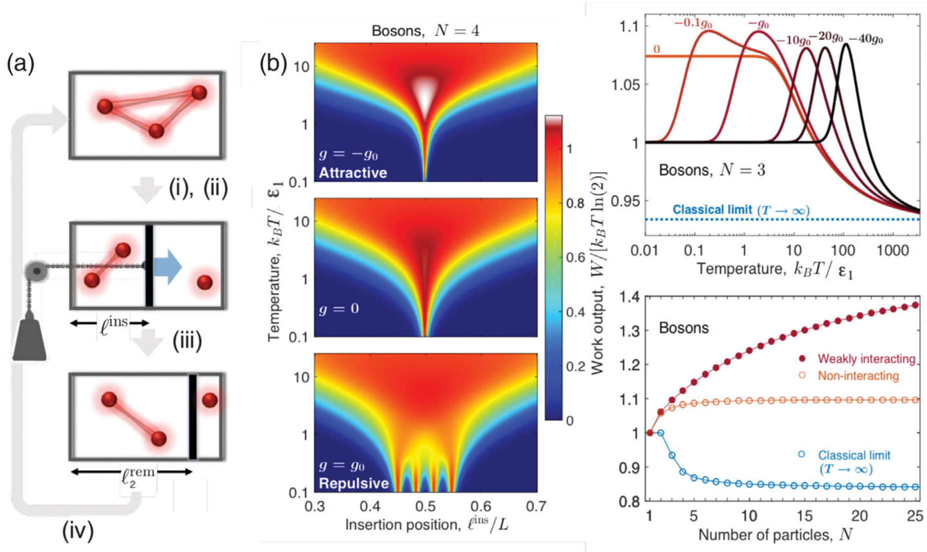

FIG. 1. Szilard engine harboring many interacting bosons in one dimension. (a) Illustration of one possible single Szilard cycle. (b) For $N=4$ bosons the optimal work output W (in units of the classical single-particle work $W_1=k_BT\ln 2$, with its magnitude illustrated by the color bar to the right) is found for attractive interactions g (upper panel) at a finite temperature and around a symmetric insertion position of the barrier. The optimal work output exceeds the case of noninteracting (middle panel) and repulsive bosons (lowest panel). (c) Work output for $N=3$ as a function of temperature for different strengths of the attractive interaction. For large T, all curves converge into the classical limit. (d) The maximal work output W/W_1 increases dramatically with the particle number for bosons with attractive interactions with $g=-0.01g_0$ (red) compared with the case for noninteracting bosons (orange) and classical particles (blue). In each case, the temperature is chosen to maximize the relative work output. Optimal insertion and removal positions of the wall are used to maximize W/W_1.

perturbative approach (see Supplemental Material [32]). Our results indicate that the output of the information-to-work conversion increases with N.

The total average work output of a single cycle with processes (i)–(iv) is given by [25]

$$W=-k_BT\sum_{n=0}^{N}p_n(\ell^{\rm ins})\ln\left(\frac{p_n(\ell^{\rm ins})}{p_n(\ell_n^{\rm rem})}\right),\qquad(1)$$

which is valid also in the classical case [34]. Here, $p_n(\ell)$ denotes the probability of n particles found to the left of the wall located at position ℓ, and $N-n$ particles to the right, if the combined system is in thermal equilibrium. The ith N-particle eigenstate $\Psi_{n,i}$ with energy $E_{n,i}$ can be classified by the particle number n in the left subsystem where $0<x<\ell$. We then find that $p_n(\ell)=\sum_i e^{-E_{n,i}(\ell)/k_BT}/Z$ with $Z=\sum_{n=0}^{N}\sum_i e^{-E_{n,i}(\ell)/k_BT}$.

Measuring the particle number on one side after insertion of the wall, one gains the Shannon entropy $I=-\sum_{n=0}^{N}p_n(\ell^{\rm ins})\ln p_n(\ell^{\rm ins})$ which measures the amount of acquired information. Going back to the original state in the cycle, the average increase of entropy $\Delta S=k_BI$ allows extracting the average amount of work $W\le k_BTI$, which can be positive. Here, the equality only holds if all $p_n(\ell_n^{\rm rem})\equiv 1$. In this case the removal of the barrier (iv) is a reversible process for each observed particle number. This reversibility had been associated with the conversion of the full information gain into work [35], as explicitly assumed in Ref. [8]. Now, $p_n(\ell_n^{\rm rem})=1$ for $\ell_0^{\rm rem}=0$ and $\ell_N^{\rm rem}=L$, as in this case all particles are on one side of the wall. Thus, for $N=1$ a full conversion of information gain to work is always possible. However, for $N\ge 2$, this does not hold any longer; e.g., there are no removal positions $\ell_1^{\rm rem}$ satisfying $p_1(\ell_1^{\rm rem})=1$ due to the finite probability of fluctuations in particle number. Similar to the noninteracting case [27], we choose the optimal $\ell_n^{\rm rem}$, maximizing $p_n(\ell_n^{\rm rem})$. We note that the extracted work for $N\ge 2$ at finite temperature is lower than the theoretical bound to the information gain k_BTI.

The full many-body solution [Figs. 1(b) and 1(c)] as well as the perturbation approach clearly demonstrates that the quantum Szilard engine with attractive bosons generates a high relative work output, peaked at nonzero temperature. This advantage is not limited to the few-body regime, but even persists for large particle numbers [Fig. 1(d)]. The average work of the $N=4$ engine has the maximum at $W/W_1\approx 1.12$ [top panel in Fig. 1(b)], which surpasses the results for noninteracting (middle panel with $W/W_1\lesssim 1.08$) as well as for repulsive bosons (lowest panel). For attractive interactions, the maximum work output always occurs if the wall is inserted in the middle of the container when the engine operates in the deep quantum regime (albeit for higher temperatures, there is a pitchfork bifurcation [36] to an asymmetric insertion position, see Supplemental Material [32]). For $T \to 0$, the work output vanishes if $\ell^{\mathrm{ins}} \neq L/2$ [Fig. 1(b)]. In this limit all noninteracting bosons occupy the lowest single-particle quantum level. After insertion of the wall, the energetically lowest-lying level is in the larger subsystem. For $\ell^{\mathrm{ins}} \neq L/2$ we thus know beforehand the location of the particles: measuring their number does not provide new information, i.e., $I = 0$. Consequently, no work can be extracted in the cycle. Attractive interactions enhance this feature. However, this does not hold for repulsive interactions, $g > 0$ [Fig. 1(b)]. In this case, the particles spread out on different sides of the wall in the ground state. Here, degeneracies between different many-particle states occur at particular values of ℓ^{ins}, which allow an information gain in the measurement. This explains the N distinct peaks as a function of ℓ^{ins} for low temperature and repulsive interactions [26,30].

The boosted information-to-work conversion of the many-body Szilard engine containing attractive bosons occurs for a wide range of interaction strengths [Fig. 1(c)]. Increasing $|g|$ not only shifts the peaks in W/W_1 to higher temperatures, but also alters their maximum value, reflecting the complexity of the spectrum of many-body excitations in the limit of stronger correlations.

The optimal relative work output [Fig. 1(d)] is higher for weakly attractive than for noninteracting bosons, as well as for the classical limit. For noninteracting bosons, we analytically show that the work output saturates at $W/W_1 \approx 1.0974$ in the limit of large N (see Supplemental Material [32]). Already in the limit of infinitesimally weak attractive interactions, a perturbative approach indicates saturation at $W/W_1 \approx 1.6$ for large N significantly exceeding the noninteracting value. For stronger interactions, however (as for example in the case with $g = 0.01 g_0$ shown in Fig. 1), the large-N behavior could not be resolved, as the perturbative approach requires interaction strengths much smaller than the order of $1/N$. Other types of (weak) attractive interactions give rise to a similar effect, as long as the corresponding interaction energy is much smaller than the level spacing.

Let us now return to the temperature dependence of W/W_1, and study the onset of the peak at an intermediate temperature. For $g < 0$, the work output equals $k_B T \ln 2$ at low temperatures, independently of N. Because of the dominance of the attractive interaction, all N particles will be found on one side of the barrier. When the barrier is inserted in the middle, we have $p_0(L/2) = p_N(L/2) = 1/2$, while all other $p_n(L/2)$ vanish. At the same time, the removal position $\ell_0^{\mathrm{rem}} = 0$ and $\ell_N^{\mathrm{rem}} = L$ provide $p_0(\ell_0^{\mathrm{rem}}) = 1$ and $p_N(\ell_N^{\mathrm{rem}}) = 1$, so that Eq. (1) provides the work output $W = k_B T \ln 2$ for the entire cycle [Fig. 1(c)]. This case, with two possible measurement outcomes and a full sweep of the piston, resembles the single-particle case. One might wonder, whether the increased particle number should not imply a higher pressure on the piston and thus, more work. This, however, is not the case, as the attraction between the particles reduces the pressure. Also, when inserting the barrier, the difference in work due to the interactions has to be taken into account. With increasing temperature (i.e., $k_B T \sim -3g(N-1)/L \approx -0.6(N-1)E_1 g/g_0$, for weak interactions) other measurement outcomes than that of all particles being on either side, i.e., $n = 0$ or $n = N$, become probable. Since $p_0(L/2)$ and $p_N(L/2)$ now decrease with temperature, we see a deviation from the performance of the single-particle engine.

To get a better understanding of the enhanced work output for attractive bosons at finite temperatures, we consider the simplest possible case with only two particles. For a central insertion of the barrier, we find $p_0(L/2) = p_2(L/2)$. For the same symmetry reasons, $p_1(\ell)$ has a maximum at this barrier position. No work can thus be extracted in cycles where the two particles are measured on different sides of the central barrier, since $p_1(\ell^{\mathrm{ins}} = L/2)/p_1(\ell_1^{\mathrm{rem}}) \geq 1$ in Eq. (1). Therefore, the only contributions to the work output result from cycles where both particles are on the same side of the barrier. Together with $p_0(\ell_0^{\mathrm{rem}} = 0) = p_2(\ell_2^{\mathrm{rem}} = L) = 1$, we obtain

$$W = -2 k_B T p_0(L/2) \ln p_0(L/2). \tag{2}$$

The maximum work output here is not obtained for the maximum Shannon entropy at $p_0(L/2) = 1/3$, setting the upper bound for the information-to-work conversion, but instead at $p_0(L/2) = 1/e$ with the value $W = (2/e) k_B T \approx 1.061 k_B T \ln 2$, see Fig. 2. This implies a finite value $p_1(L/2) = 1\text{–}2/e$. Even if no work can be extracted with one particle on either side of the barrier, a nonzero probability $p_1(L/2)$ of such a measurement outcome can be preferable, contributing to the information.

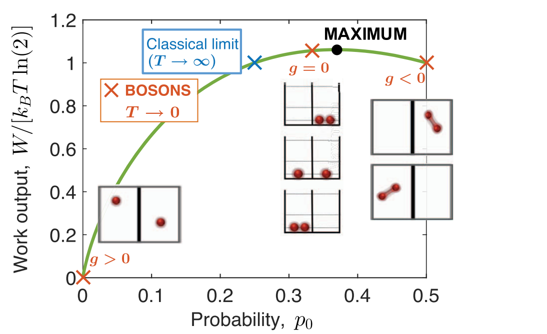

FIG. 2. Work output per cycle for the two-particle Szilard engine. For a symmetric insertion of the barrier the work output depends solely on the probability p_0 to find all particles on the right side. For $T \to \infty$, $p_0 = 1/4$. In the limit of low temperature, p_0 differs for bosons with different interactions. It moves from the red to the blue cross with increasing T. The insets show the ground state degeneracies for noninteracting (middle), repulsive (left), and attractive bosons (right).

Two attractive bosons, initially at $T \to 0$ and with $p_0(L/2) = 1/2$, will continuously approach the classical limit of $p_0(L/2) = 1/4$ as T increases. Hence, at a certain temperature, depending on the interaction strength, $p_0(L/2)$ passes through $p_0(L/2) = 1/e$ producing a maximum in the relative work, as seen in Fig. 2. One may understand this as follows: At low temperatures, the two attractive bosons will always end up on the same side of the barrier, bound together by their attraction. The cycle then operates similarly to the single-particle case, which explains why $W = k_B T \ln 2$ when $p_0(L/2) = 1/2$. A less correlated system (obtained with increasing T) provides a larger expansion work for cycles in which both particles are on one side of the barrier. On the other hand, cycles with one particle on each side of the barrier, from which no work can be extracted, become more common. For $1/e < p_0(L/2) < 1/2$, the enhanced pressure is more important and the average work output increases with decreasing $p_0(L/2)$. For lower values of $p_0(L/2)$, i.e., $p_0(L/2) < 1/e$, too few cycles contribute on average to the work production. The average work output therefore decreases with decreasing $p_0(L/2)$ despite the corresponding increase in pressure. Importantly, we note the absence of a similar maximum in the noninteracting case, where W/W_1 is found to decrease steadily towards the classical limit with increasing T.

Let us now proceed to the more complicated case of $N > 2$ attractive bosons. Also here we observe a pronounced maximum in W/W_1 (see Fig. 1c), going from the attractive to the noninteracting regime by increasing T. Similar to the two-particle engine, the combined contribution to the average work output from cycles in which all particles are on the same side of the barrier inserted at $\ell^{\text{ins}} = L/2$ is given by Eq. (2). For all interaction strengths $g < 0$, the peak height is consequently at least equivalent to the maximum work of the attractive two-particle case $W_2 \approx 1.061 k_B T \ln(2)$ obtained with $p_0(L/2) = 1/e$. This is due to the fact that $p_0(L/2)$ necessarily decreases from 1/2 at $T \to 0$ to the classical result $1/2^N$ at large temperatures, going through the value of $1/e$. In general, also cycles with $n = 1, 2, \ldots, N-1$ (except if $n = N/2$) on the left side of the barrier contribute to the average work output, which therefore can be even higher than in the two-particle case. For example, for $N = 4$, the maximum of $p_1(\ell)$ and that of $p_3(\ell)$ occurs for $\ell \neq L/2$, as shown by the probabilities for different measurement outcomes in Fig. 3. In this case, ℓ_n^{rem} can be chosen such that $p_n(\ell^{\text{ins}})/p_n(\ell_n^{\text{rem}}) < 1$ for $\ell^{\text{ins}} = L/2$ and work may be extracted in agreement with Eq. (1). With insertion of the barrier at the midpoint the relative work W/W_1 is maximized for $p_0(L/2) = p_4(L/2) \approx 0.3$, a number that is close to the optimal value $1/e$ for the corresponding two-particle engine. However, there are smaller contributions, here for $n = 1$ and $n = 3$, that one needs to take into account in order to optimize the engine. With increased N, the contribution from cycles in which $1 \leq n \leq N-1$ becomes of greater importance in the optimization of the information-to-work conversion. The probability $p_0(\ell^{\text{ins}}/L)$ at the maximum of W/W_1, is here seen to shift slightly and move further away from the two-particle value of $1/e$ as N increases from $N = 4$ to $N = 8$ (Fig. 3.)

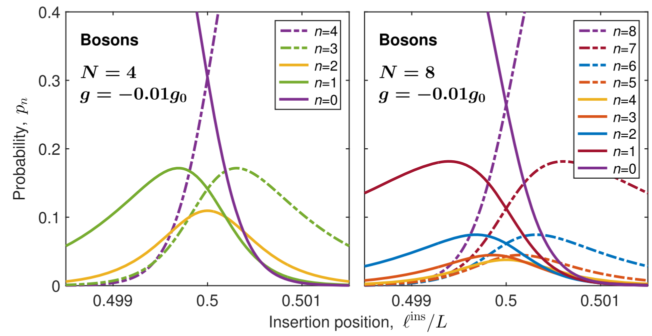

FIG. 3. Probability distributions. Work can be extracted in all cycles with insertion of the wall at the midpoint, except for the case with an equal number of particles on either side. Shown are the probability distributions assigned to the different measurement outcomes at the temperature of the maximal relative work output for $N = 4$ ($k_B T/E_1 \approx 0.243$, left panel) and $N = 8$ ($k_B T/E_1 \approx 0.0500$, right panel) bosons with weak attraction, $g = -0.01 g_0$.

Finally, let us consider repulsive contact interactions between the bosons [Fig. 1(b)]. In the low-temperature limit, the relative work output is very similar to that of noninteracting spin-polarized fermions discussed in Refs. [26,30]. This resemblance becomes even more pronounced with increasing interaction strength. This is no coincidence, but intriguingly caused by the transition into the Tonks-Girardeau regime [37], where bosons with strong, repulsive interactions that have an impenetrable core act like spin-polarized noninteracting fermions.

We conclude that the interacting quantum many-body Szilard cycle may serve as a new prototype to study the fundamental, and hitherto largely unexplored, relations between correlations, information, and thermal fluctuations in a wide range of quantum many-body systems. A possible experimental realization could be with cold atoms, as already suggested in Refs. [8,25], where stronger correlations [31] and the few-body regime [38] can be realized. Another example are polariton condensates [39]. Note that in a realistic setup, there are many sources for noise that may deteriorate the information-to-work conversion, such as inaccurate configuration measurements, impurities, tunneling due to a finite-height barrier and, inevitably, thermal noise due to the coupling to the heat bath. Measurement errors and imperfect feedback control are discussed e.g., in the review [40], and very recently for a realistic single-electron setup in Ref. [41]. We here restrict our analysis to idealized quasistatic processes. It would be of much interest to consider a finite speed in the motion of the piston (similar to what has been investigated recently for quantum Otto engines [42,43]). A great future challenge will be to quantify irreversibility in real processes on the basis of a fully *ab initio* quantum description, which may allow us to study dissipative aspects in the kinetics of the conversion between information and work [19]. A particularly exciting perspective has very recently been opened up by Ref. [20], discussing the emergence of thermal fluctuations from quantum fluctuations for isolated many-body systems.

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