Autonomous circular heat engine

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A dynamical model of a highly efficient heat engine is proposed, where an applied temperature difference maintains the motion of particles around the circuit consisting of two asymmetric narrow channels, in one of which the current flows against the applied thermodynamic forces. Numerical simulations and linear-response analysis suggest that, in the absence of frictional losses, the Carnot efficiency can be achieved in the thermodynamic limit.

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I. INTRODUCTION

In the past decades, studying classical and quantum transport from the microscopic dynamics perspective has led to major advances in our understanding of heat conduction in low-dimensional systems [1-8], unveiling fundamental mechanisms of normal and anomalous transport and the conditions for heat rectification. In more recent years, investigations have been extended to more complicated situations involving two or more coupled currents, like in thermoelectric [9] or thermodiffusive [10] transport. Also in this case, a microscopic approach has played a unique role, finding new paths to achieve the Carnot efficiency in heat-to-work conversion [11,12], extending Onsager reciprocal relations to systems with broken time-reversal symmetry [13,14], and discovering the highly counterintuitive phenomenon of inverse currents, whereby an induced current flows opposite to the applied thermodynamic forces [15–17].

We propose to extend these notions to mass transport in low dimensional geometries, like narrow channels, where particles tend to move in single-files [18]. Indeed, when their diameter is comparable to the channel cross section, particles either do not pass each other at all, or do so only by overcoming a repulsive potential barrier and, possibly, at the cost of frictional losses [19]. However, single files subject to thermal gradient not only pose a fundamental problem for themselves (with potential applications to natural and artificial nanodevices [18]) but can also be suitably arranged to produce coupled particle currents.

Here, we demonstrate the possibility of building a circular heat engine consisting of two channels coupled to two particle reservoirs maintained at different temperatures. In

addition, each channel contains particles of a different species, which either repel or bypass the particle flowing between the reservoirs, depending on their masses and velocities. For an appropriate choice of these parameters, the particle current in one channel may flow from low to high temperatures, and a stationary circular current between the reservoirs is established. As a consequence, the engine can convert a substantial fraction of the heat flowing from the hot to the cold reservoir into work. Extensive numerical simulations and a linear-response analysis suggest that the Carnot efficiency can indeed be achieved in the thermodynamic limit, i.e., for infinitely long channels.

II. MODEL AND ENGINE MECHANISM

A sketch of the proposed engine is plotted in Fig. 1. It is made of two one-dimensional (1D) channels of length L_{Ξ} $(\Xi = A, B)$, coupled at their end points to two reservoirs of temperatures T_k (k = L, R). The number of particles in the overall system (channels plus reservoirs) is fixed. Each channel contains two species of particles, graphically represented by bullets of mass m and rods of mass M_{Ξ} , respectively. Dynamics inside the channels is purely Hamiltonian. All particles move freely, except when they collide with one another or hit a channel end point. When two particles collide, they either pass through each other, if their total energy in the frame of their center of mass is larger than a fixed inner potential barrier h_{Ξ} or simply bounce back; in both cases the pair momentum and the pair kinetic energy are conserved. The particle dynamics adopted here is inspired to well-known models for single-file diffusion and granular fluids, where



FIG. 1. Sketch of a two-channel engine working between two reservoirs of fixed temperatures T_L and T_R and adjustable chemical potentials μ_L and μ_R . The two particle species in each channel are represented by bullets of mass *m* and rods of mass $M_{A,B}$. When a stationary circular current of bullets is established, the engine can work against applied potentials $U_{A,B}$. In this drawing, the channels have equal lengths, $L_A = L_B$.

 h_{Ξ} can be regarded as the energy barriers associated with the configurational changes two particles undergo whereas passing each other in the channel [18,20,21]. For the engine to work it is essential that the rods in the two channels are different. When a rod hits a channel-reservoir boundary, it is reflected back with a newly assigned velocity sampled from a certain distribution determined by the reservoir temperature (see below). Accordingly, the number of rods in each channel is conserved as they only exchange energy with the reservoirs. As for the bullets, when one reaches a channel boundary, it will enter the connected reservoir. Meanwhile, the reservoirs keep injecting bullets into the channels with rates and energy distributions determined by their temperatures T_k and densities (or chemical potentials μ_k). Following these simple rules, after an appropriate transient, a steady-state circular current of bullets sets in, sustained by the temperature difference imposed by the reservoirs; the bullet densities (and the chemical potentials μ_k) in each (large but finite) reservoir autonomously adjust to support such a current. Ultimately, the circulating particle current and, thus, the possibility of extracting useful work depend on the fixed temperature difference between the reservoirs.

Suppose that $T_L > T_R$ and $\mu_L > \mu_R$. Intuitively, we may expect that in each channel, both the energy and the bullet current would flow forward from left to right. This is indeed the case when $M_{\Xi} > m$. In sharp contrast, for $M_{\Xi} < m$ either the energy or the bullet current—depending on the parameter choice—may flow on reverse from right to left, against both thermodynamical forces [16]. The mechanism of current reversal is related to the fact that under the given collision rules, the probability for a bullet-rod pair to cross each other is higher when the light (heavy) particle is on the hot (cold) reservoir side because in such a case, their relative velocities are likely to be higher. The kinetics of bullets and rods, thus, causes a left-right unbalance in their densities along the channel [22].

Thanks to this peculiar dynamical effect, we can make the bullets flow on reverse in one channel, say, channel *B*, by setting $M_B < m$ and, thus, create a clockwise circular bullet

current through the whole system. Such current can work also against an external bias, represented by the potentials $U_{A,B}$ in Fig. 1 [23]. For instance, one could use part of the kinetic energy of the circulating particles to lift a weight. A fraction of the heat flowing from the hot to the cold reservoir would be then converted into mechanical work, the rest being dumped into the cold reservoir. This fulfills the function of an engine.

III. LINEAR-RESPONSE ANALYSIS

Before presenting the output of our numerical simulations, we analyze the model in the linear-response regime. We adopt here for concreteness the language of thermoelectricity, with charged particles circulating, such as in a thermocouple, but our results apply equally well to other coupled flows, such as in thermodiffusion. We start from the linear transport equations [24,25] for channel Ξ ($\Xi = A, B$),

$$\begin{pmatrix} J_{\Xi}^{\rho} \\ J_{\Xi}^{u} \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{\Xi}^{\rho\rho} & \mathcal{L}_{\Xi}^{\rhou} \\ \mathcal{L}_{\Xi}^{u\rho} & \mathcal{L}_{\Xi}^{uu} \end{pmatrix} \begin{pmatrix} \mathcal{F}_{\Xi}^{\rho}/L_{\Xi} \\ \mathcal{F}^{u}/L_{\Xi} \end{pmatrix}.$$
 (1)

Here J_{Ξ}^{ρ} and J_{Ξ}^{u} are the particle (bullet) and the energy currents, $\mathbb{L}_{\Xi} = (\mathcal{L}_{\Xi}^{ij})$ $(i, j = \rho, u)$ the matrix of the Onsager kinetic coefficients, and \mathcal{F}_{Ξ}^{ρ} and \mathcal{F}^{u} the thermodynamical forces, defined as $\mathcal{F}_{A}^{\rho} = \mu_{L}\beta_{L} - (\mu_{R} + U_{A})\beta_{R}$, $\mathcal{F}_{B}^{\rho} = \mu_{L}\beta_{L} - (\mu_{R} - U_{B})\beta_{R}$, and $\mathcal{F}^{u} = \beta_{R} - \beta_{L}$, respectively, with $\beta_{k} = 1/(k_{B}T_{k})$ $(k = L, R, k_{B}$ is the Boltzmann constant). The Onsager coefficients are related with the familiar transport coefficients, i.e., the electrical conductivity σ_{Ξ} , the thermal conductivity κ_{Ξ} , and the thermopower S_{Ξ} as follows:

$$\sigma_{\Xi} = \frac{e^2}{T} L_{\Xi}^{\rho\rho}, \quad \kappa_{\Xi} = \frac{1}{T^2} \frac{\det \mathbb{L}_{\Xi}}{L_{\Xi}^{\rho\rho}}, \quad S_{\Xi} = \frac{1}{eT} \left(\frac{L_{\Xi}^{\rho u}}{L_{\Xi}^{\rho\rho}} - \mu \right),$$
(2)

where *e* is the charge of each particle, $T \approx T_L \approx T_R$, $\mu \approx \mu_L \approx \mu_R$ in linear-response approximation. We can then rewrite Eq. (1) as

$$\begin{split} L_A J_A^u &= \kappa_A' \Delta T + T \sigma_A S_A (\Delta \mu - U_A), \\ L_B J_B^u &= \kappa_B' \Delta T + T \sigma_B S_B (\Delta \mu + U_B), \\ L_A J_A^\rho &= \sigma_A S_A \Delta T + \sigma_A (\Delta \mu - U_A), \\ L_B J_B^\rho &= \sigma_B S_B \Delta T + \sigma_B (\Delta \mu + U_B). \end{split}$$

Here $\kappa'_A = \kappa_A + T \sigma_A S_A^2$, $\kappa'_B = \kappa_B + T \sigma_B S_B^2$, $\Delta T = T_L - T_R$, and $\Delta \mu = \mu_L - \mu_R$. On imposing the circular steady-flow condition,

$$J_A^{\rho} + J_B^{\rho} = 0, (3)$$

the output power P and the efficiency η read, respectively,

$$P = J_A^{\rho} U_A - J_B^{\rho} U_B, \quad \eta = P/(J_A^{u} + J_B^{u}).$$
(4)

Note that by using the steady-flow condition, P and η can be explicitly rewritten as functions of $U_A + U_B$, rather than of U_A and U_B , separately (see Appendix A). Moreover, both the maximum efficiency η_{max} and the efficiency at the maximum power $\eta(P_{\text{max}})$ have the usual dependence [9] on a nondimensional figure of merit,

$$YT = \frac{(\sigma_A/L_A)(\sigma_B/L_B)(S_A - S_B)^2}{(\sigma_A/L_A + \sigma_B/L_B)(\kappa_A/L_A + \kappa_B/L_B)}T,$$
 (5)

(in lieu of the thermoelectric figure of merit ZT [26,27]), namely,

$$\eta_{\max} = \eta_C \frac{\sqrt{YT+1}-1}{\sqrt{YT+1}+1}, \quad \eta(P_{\max}) = \frac{\eta_C}{2} \frac{YT}{YT+2}, \quad (6)$$

with Carnot efficiency $\eta_C = 1 - T_R/T_L$ (we assume $T_L > T_R$) and maximum power,

$$P_{\max} = \frac{1}{4} \frac{\sigma_A \sigma_B}{\sigma_A L_B + \sigma_B L_A} (S_A - S_B)^2 (\Delta T)^2.$$

The power-efficiency trade-off for a given value of YT can also be obtained (see, e.g., Ref. [9]),

$$\frac{\eta}{\eta_C} = \frac{P/P_{\text{max}}}{2[1+2/(YT) \mp \sqrt{1-P/P_{\text{max}}}]}.$$
 (7)

A limiting case is represented by the conventional thermocouple configuration with $L_A = L_B \equiv L$, $\sigma_A = \sigma_B \equiv \sigma$, $\kappa_A =$ $\kappa_B \equiv \kappa$, and $S_A = -S_B \equiv S$. Here, the figure of merit ZT is recovered, ZT = YT, and the maximum power $P_{\text{max}} =$ $(\sigma/2L)S^2(\Delta T)^2$ amounts to twice the maximum power of a single channel.

IV. NUMERICAL STUDY

Our numerical results show that the proposed engine is very efficient. In our simulations, we model the reservoirs as 1D ideal gases of bullets [28]. They inject bullets into the channels randomly in time with constant rates $\gamma_k \ (k = L, R) \ [29], \ \gamma_k = (\rho_0 / \sqrt{2\pi m \beta_0}) (\beta_0 / \beta_k) e^{\mu_k \beta_k - \mu_0 \beta_0},$ where $T_0 = 1/(k_B \beta_0)$, ρ_0 , and μ_0 are, respectively, the temperature, particle number density, and chemical potential of a reference state (see below). The injection intervals, thus, follow the Poisson distribution $\pi_k(t) = \gamma_k e^{-\gamma_k t}$, whereas the speeds of the injected particles are sampled according to the Maxwell distribution [30], $P_k(v, m) = m|v|\beta_k e^{-mv^2\beta_k/2}$. Accordingly, when a rod particle of mass M_{Ξ} hits the channel boundary next to reservoir k, it bounces back with speed distribution $P_k(v, M_{\Xi})$.

To establish the circular steady-flow condition of Eq. (3), rather than simulating the entire closed system (that is, channels and reservoirs), we simulated first the two channels, separately, and computed the two curves J_{Ξ}^{ρ} vs U_{Ξ} ($\Xi = A, B$). Then, for a given value of $J^{\rho} \equiv J_A^{\rho} = -J_B^{\rho}$, we determined the corresponding values of $U_{A,B}$, to be used in the subsequent simulation steps, which involve both channels simultaneously. After the system had relaxed to its stationary state, we computed the time-averaged currents and from Eqs. (4), the relevant output power P and the efficiency η .

In the simulations reported here, we set $T_L = T + \Delta T/2$, $\mu_L = \mu + \Delta \mu/2$, $T_R = T - \Delta T/2$, and $\mu_R = \mu - \Delta \mu/2$. The number of rods in each channel is set to half of the expected particle number of a 1D ideal gas at the equilibrium with the assigned T and μ , i.e., $N_{\text{rod},\Xi} = \rho L_{\Xi}/2$ with $\rho =$ $\rho_0 \sqrt{\beta_0/\beta} e^{\beta \mu - \beta_0 \mu_0}$. As for the reference state, we set $\rho_0 = 1$, $T_0 = 1$, and $\mu_0 = 0$ (in units such that m = 1, e = 1, and $k_B = 1$). To make the system evolve in time, we implemented an effective event-driven algorithm [31], which yields output data points with relative error less than 0.5%.

Our data show that this model works as an autonomous engine in a wide range of parameters. Typical numerical results

 $\delta/10^{-5}$ 0



0.6

FIG. 2. (a) Efficiency, η , vs output power P for two channels of equal length $L_A = L_B$. Blue dots, red squares, blue diamonds, and green triangles are for $L_{\Xi} = 100, 200, 400, \text{ and } 1600, \text{ respectively.}$ The curves next to each data set are obtained via Eq. (7) with numerically computed YT. Fixed model parameters are as follows: $h_A = h_B = 1, M_A = 1.5, M_B = 0.5, T = 1$, and $\mu = 1.5$; Other tunable parameters are $\Delta T = 0.1$ and $\Delta \mu = 0.15$. (b) η vs P, such as in (a), for $L_{\Xi} = 200$ but finite dissipation parameter δ (see the text below).

for the efficiency and the power are displayed in Fig. 2(a), where for any given system size $L_A = L_B$, a data point represents the result obtained for a certain value of J^{ρ} (or U_A and U_B). The closed curve next to each set of the data points is the prediction of Eq. (7), plotted for the corresponding value of YT, also obtained by numerical simulation as explained below. The linear-response theory reproduces quite closely the numerical data of Fig. 2(a). Moreover, such agreement improves with increasing the system size as expected since the temperature gradient $(\nabla T)_{\Xi} = \Delta T/L_{\Xi}$, decreases upon increasing L_{Ξ} at constant ΔT . More importantly, we note that as L_{Ξ} increases, the efficiency vs power curves shift upwards, meaning that the engine performance improves. This remark hints at the possibility that the figure of merit YT in Eq. (7) is a monotonically increasing function of the system size.

To determine YT we made use of Eq. (5), where the transport coefficients are also to be computed numerically. To this purpose, the two channels were considered separately. For each channel, we followed the method detailed in Ref. [29], i.e., the particle and energy currents were measured twice, namely, for $\mathcal{F}_{\Xi}^{\rho} \neq 0$ and $\mathcal{F}^{u} = 0$, and for $\mathcal{F}_{\Xi}^{\rho} = 0$ and $\mathcal{F}^{u} \neq 0$ (having set $U_{\Xi} = 0$). The Onsager kinetic coefficients can then be evaluated through Eq. (1). The corresponding transport coefficients Eq. (2), computed for three different potential barrier values, $h_A = h_B = 0.5$, 1.0, and 1.5, are displayed in Figs. 3(a)-3(c) vs L_{Ξ} . First of all, we note that due to the inverse bullet current in channel B, the off-diagonal elements of the Onsager matrix are negative [16,32]. Accordingly, the Seebeck coefficients S_A and S_B are, respectively, positive and negative [see Fig. 3(a)], which enhances the figure of merit YT through the quadratic factor $(S_A - S_B)^2$ in Eq. (5). This is the key advantage of our model. Moreover, due to the fact that the momentum is the only conserved mechanical quantity both S_{Ξ} and factor $(S_A - S_B)^2$ in our expression for *YT* are predicted to saturate in the thermodynamic limit [12], a prediction corroborated by our numerical simulations.



FIG. 3. (a)–(c) Transport coefficients of the two channels vs their lengths where the empty and the full symbols are for channel *A* and channel *B*, respectively. (d) *YT* versus $L_A = L_B \equiv L$ for $h_A = h_B$. In all four panels, green squares, blue dots, and red triangles are for, respectively, $h_{\Xi} = 0.5$, 1.0, and 1.5, All other simulation parameters are the same as in Fig. 2(a).

As for the electrical and thermal conductivities, it helps consider two limits for the potential barriers h_{Ξ} . In the limit $h_{\Xi} \rightarrow \infty$, all particles turn out to be hard core and the two species in each channel are always nonpassing. The bullet currents are, therefore, blocked, thus, resulting in $\sigma_{\Xi} = 0$. On the other hand, according to the 1D heat conduction theory [3,4,33,34], in the thermodynamical limit the heat conductivity would diverge, such as $\kappa_{\Xi} \sim L_{\Xi}^{\nu}$ with $0 < \nu < 1$. Consequently, see Eq. (5), in the same limit both YT and the engine efficiency would vanish. In the opposite limit $h_{\Xi} \rightarrow 0$ the dynamics becomes integrable, and the bullets flow through the channel freely; hence, $\sigma_{\Xi} \sim L_{\Xi}$ and $\kappa_{\Xi} \sim L_{\Xi}$. This working regime is not advantageous either. Indeed, the bullet-rod interaction is crucial to maintain an inverse current [16] in channel B. Therefore, when the bullet-rod interaction vanishes for $h_B \rightarrow 0$, so does the inverse current. More precisely, there exists a critical value h_B^* such that for $h_B < h_B^*$, the bullet current in channel Bstarts flowing forward, and our engine, thus, stops working. Note that $h_B^* \sim L_B^{-0.5}$ (see Appendix B) so that $h_B^* \to 0$ as $L_B \to \infty$. It is, therefore, reasonable to conjecture that for a given system size, one can determine the optimal finite values of h_{Ξ} that maximize YT.

Based on the data in Figs. 3(a)-3(c), we can investigate how *YT* depends on the system size for assigned values of h_{Ξ} . We find that, in general, when $L_A + L_B$ is fixed, *YT* reaches its maximum for $L_A \simeq L_B$ and $h_A = h_B$. For this reason, we focus on cases with $L_A = L_B$ and $h_A = h_B$, and in Fig. 3(d) plot *YT* vs L_{Ξ} for three values of h_{Ξ} . *YT* is confirmed to be an increasing function of L_{Ξ} , which saturates asymptotically to a value that increases as h_{Ξ} decreases. In addition, the optimal h_{Ξ} value that for a given L_{Ξ} maximizes *YT* decreases as L_{Ξ} increases [from Fig. 3(d), we can tell that the optimal h_{Ξ} value is larger than one for $L_{\Xi} < 150$ but smaller than one for $L_{\Xi} > 4000$]. Based on the numerical and analytical results reported above, we conjecture that the engine achieves the Carnot efficiency (corresponding for $YT \to \infty$ to the values of bias potentials $U_{A,B}$ for which the efficiency is maximum, transport is dissipationless and power vanishes [9]) in the thermodynamic limit $L_{\Xi} \to \infty$ and for vanishing barriers $h_{\Xi} \sim 1/\sqrt{L_{\Xi}} \to 0$.

Of course, this conclusion holds under the condition that the dynamics in both channels is frictionless. Two particles in a single file (say, a bullet and a rod) do squeeze their way past each other when their relative velocity $|v_{i+1} - v_i|$ is large enough to overcome the relevant repulsive barrier h_{Ξ} . However, the collisional mechanism may involve the loss of a fraction of their kinetic energy. Accordingly, imposing pair momentum conservation, the respective momentum changes would be $\Delta p_i = -\Delta p_{i+1} = \delta/(v_i - v_{i+1})$ with δ the assumed dissipation parameter. Such a simple collisional friction model impacts the backward current in channel *B* more than the forward current in channel *A*; this results in the net suppression of the power-efficiency performance of the engine illustrated in Fig. 2(b).

V. SUMMARY AND DISCUSSION

We have exploited the phenomenon of inverse particle current to design an autonomous engine, which for a given temperature difference, operates without any external time-dependent control. When operated on reverse, this engine would work as a refrigerator. The linear-response analysis outlined above shows that the engine performance would still be governed by *YT* with maximum efficiency as in Eq. (6) but with reversed Carnot coefficient $\eta_C = (T_L/T_R - 1)^{-1}$. Finally, due to its peculiar nature, distinct from the conventional steady-state engines characterized by *ZT*, our engine can be used to investigate the trade-off of power, efficiency, and fluctuations, encompassed in thermodynamic uncertainty relations [35–38].

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APPENDIX A: DEPENDENCE OF POWER AND EFFICIENCY ON $U_A + U_B$

Given the currents [see the four equations before Eq. (3)] for the currents, and the steady-flow condition $J_A^{\rho} + J_B^{\rho} = 0$, we obtain

$$J_A^{\rho} = -J_B^{\rho} = \frac{1}{2} \left(J_A^{\rho} - J_B^{\rho} \right) = \frac{1}{2} \left[\left(\frac{\sigma_A S_A}{L_A} - \frac{\sigma_B S_B}{L_B} \right) \Delta T + \left(\frac{\sigma_A}{L_A} - \frac{\sigma_B}{L_B} \right) \Delta \mu - \left(U_A + U_B \right) \right],$$
(A1)



FIG. 4. Dependence of the current J_B^{ρ} on the potential barrier h_B for $M_B = 0.5$, T = 1, $\mu = 1.5$, $\Delta T = 0.1$, and $\Delta \mu = 0$.

where the last equality is obtained by substituting J_A^{ρ} and J_B^{ρ} . This expression shows that both J_A^{ρ} and J_B^{ρ} depend on $U_A + U_B$, rather than on U_A and U_B , separately. Moreover, as

$$P = J_A^{\rho} U_A - J_B^{\rho} U_B = J_A^{\rho} (U_A + U_B),$$
 (A2)

we conclude that the power depends on $U_A + U_B$ as well. On the other hand, by eliminating $\sigma_A(\Delta \mu - U_A)$ and $\sigma_B(\Delta \mu + U_B)$ based on the four equations before Eq. (3), we have that

$$J_A^u = T S_A J_A^\rho + \kappa_A \Delta T / L_A,$$

$$J_B^u = T S_B J_B^\rho + \kappa_B \Delta T / L_B.$$
 (A3)

It follows that J_A^u and J_B^u , and, in turn, the efficiency, also

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FIG. 5. Dependence of the critical potential barrier h_B^* , obtained from the data of Fig. 4, on the channel length L_B .

depend on $U_A + U_B$ alone. In conclusion, as long as their sum is kept constant, we can vary U_A and U_B without modifying power and efficiency.

APPENDIX B: CRITICAL VALUE FOR THE POTENTIAL BARRIER

There exists a critical value h_B^* such that for $h_B < h_B^*$, the bullet current in channel *B* starts flowing forward and the engine, thus, stops working. In the main text it was stated that $h_B^* \sim L_B^{-0.5}$. This is a very accurate numerical observation. Figure 4 shows the dependence of the particle current J_B^{ρ} on the potential barrier h_B for various channel lengths L_B . For a given value of L_B , the critical potential value h_B^* is identified by interpolating data points and solving $J_B^{\rho}(h_B^*) = 0$. We can see from Fig. 5 that the obtained values of the critical potential barrier are in excellent agreement with the scaling $h_B^* \sim L_B^{\alpha}$ with $\alpha = -0.500 \pm 0.004$.

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BENENTI, CASATI, MARCHESONI, AND WANG

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