Comment on "Dynamically induced heat rectification in quantum systems"

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The article by Riera-Campeny, Mehboudi, Pons, and Sanpera [Phys. Rev. E **99**, 032126 (2019)] studies heat rectification in a network of harmonic oscillators which is periodically driven. Both the title and introduction stress the quantum nature of the system. Here we show that the results are more general and are equally valid for a classical system, which broadens the interest of the paper and may suggest further pathways for a basic understanding of the phenomenon.

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Reference [1] investigates a new mechanism to induce heat rectification in a physical system. In analogy to electrical diodes, a thermal diode, which connects two thermal baths at different temperatures, exhibits different thermal conductivities if the temperatures of the baths are exchanged. Earlier studies considered static systems, i.e., systems with time-independent properties and some nonlinearity in the physics of the material. Theory has considered classical and quantum systems. In these static systems the basic origin of heat rectification can simply be tracked down in some asymmetry in the design of the device and in the temperature dependence of the thermal conductivity of the material [2]. Heat rectifiers have been built [3] based on this simple idea. The concept introduced in Ref. [1] is different because the authors consider a system under generic *linear* interactions, but they introduce some internal dynamics in the device with time-dependent interactions. This is an interesting idea and Ref. [1] shows that it is valid in a large variety of configurations. Dynamic rectification had already been considered in optics using a spatially and temporarilly modulation of the index [4]; however, the context was different because integrated photonics applications work with deterministic signals in a limited bandwidth. Thermal rectification is more challenging, and this is why the results of Ref. [1] are significant.

However, in their title and in the Introduction and Conclusion of their paper, the authors stress the quantum nature of their analysis, which gives the impression that the phenomenon that they exhibit is purely quantum. This is misleading. Actually the results are equally valid for a classical system, as in the optical case [4]. An analytical treatment is harder in this case but a numerical simulation of the classical equivalent of the simple example studied in details in Ref. [1] shows that the results of the article are preserved for the classical system. This broadens the interest of the article by showing its generic validity.

To illustrate its general results with a specific case, Ref. [1] studied a network of two oscillators, which is schematically shown in Fig. 1. Its Hamiltonian is

$$H_s(t) = \frac{1}{2m}\left(P_1^2 + P_2^2\right) + \frac{1}{2}C_1(t)X_1^2 + \frac{1}{2}C_2X_2^2 + \frac{1}{2}C_0(X_1 - X_2)^2, \quad (1)$$

where X_2 and X_2 are the positions of the oscillators, P_1 and P_2 their momenta, $C_1(t) = \omega_1^2 + 2v_1 \sin \omega_d t$ is a time-dependent parameter which introduces a driving at frequency ω_d, while $C_2 = \omega_2^2$ and C_0 are constants. This system is coupled to two thermostats, Th_1 and Th_2, at two different temperatures that we label T_h (for the highest) and T_l (for the lowest). Reference [1] investigated this system using a quantum formalism and showed that it does exhibit some thermal rectification when the temperatures T_h and T_l are switched. The results are displayed in Fig. 3 of the paper for $\omega_1^2 = 2\omega_0^2$ [5], $\omega_2 = \omega_0$, $T_h = 1.2\, T_l$, and $v_1 = 0.1$, for a range of C_0 and ω_d values.

To compare the quantum and classical properties of the system, we investigated it with the same parameters using numerical simulations in which the oscillators are treated as Langevin oscillators. This is achieved by adding damping forces $-m\gamma \dot{X}_i$ $(i = 1, 2)$ and fluctuating terms $m\Gamma_i(t)$ to the Hamiltonian equations of motions, where $\dot{X}_i = dX_i/dt$ and $\Gamma_i(t)$ is a Gaussian random variable such as $\langle \Gamma_i(t)\Gamma_i(t')\rangle = q_i\delta(t - t')$ [$\delta(t)$ is the Dirac delta function] and $q_i = 2\gamma T_i/m$, T_i being the temperature (T_h or T_l) of the thermostat connected to oscillator i, expressed in energy units. These classical equations have been integrated with the Greenside-Helfand numerical scheme for stochastic differential equations [6]. Thermal rectification was investigated with two series of numerical experiments for each set of system parameters. In the first series of realizations, thermostat Th_1 connected to oscillator X_1 was set to the high temperature T_h and thermostat Th_2 was set to T_l. Reverse configurations, marked by the exponent r, were obtained by switching T_h and T_l. Each series comprised 200 realizations, which were used to compute averages over the statistical realizations and over more than 2.5×10^5 periods $2\pi/\omega_d$, designated by $\langle\cdot\rangle$.

In the simulations, to compute the heat powers $\dot{Q}_1$ and $\dot{Q}_2$ flowing into the systems from thermostats Th_1 and Th_2, it is

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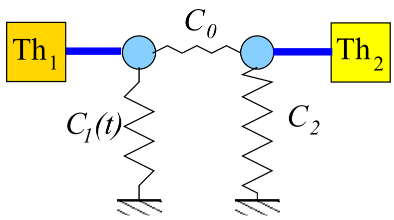

FIG. 1. Schematic picture of the simple device studied in Ref. [1].

convenient to introduce the local energies, corresponding to each of the oscillators, defined as

$$E_1(t) = \frac{P_1^2}{2m} + \frac{1}{2}C_1(t)X_1^2 + \frac{1}{4}C_0(X_1 - X_2)^2, \tag{2}$$

$$E_2(t) = \frac{P_2^2}{2m} + \frac{1}{2}C_2X_2^2 + \frac{1}{4}C_0(X_1 - X_2)^2, \tag{3}$$

so that $H_S(t) = E_1 + E_2$. Using the Hamiltonian equations of motion and taking into account the exchanges with the thermostats leads to

$$\frac{dE_1}{dt} = \dot{W}_1 - \frac{1}{2}C_0(X_1 - X_2)\left(\frac{dX_1}{dt} + \frac{dX_2}{dt}\right) + \dot{Q}_1, \tag{4}$$

$$\frac{dE_2}{dt} = \frac{1}{2}C_0(X_1 - X_2)\left(\frac{dX_1}{dt} + \frac{dX_2}{dt}\right) + \dot{Q}_2, \tag{5}$$

where $\dot{W}_1 = v_1\omega_d X_1^2 \cos\omega_d t$ is the power flowing toward oscillator 1 due to the modulation of $C_1(t)$. From the dynamical trajectories of the oscillators, dE_1/dt, dE_2/dt, $\dot{W}_1$, and $\frac{1}{2}C_0(X_1 - X_2)(\frac{dX_1}{dt} + \frac{dX_2}{dt})$ are easy to compute, which determines $\dot{Q}_1$ and $\dot{Q}_2$.

The rectification coefficient defined in Ref. [1] is derived from the fluxes $\dot{Q}_1$ and $\dot{Q}_1^r$ in the direct and reverse configurations

$$R_Q = \frac{|\langle\dot{Q}_1\rangle + \langle\dot{Q}_1^r\rangle|}{\max\left(|\langle\dot{Q}_1\rangle|, |\langle\dot{Q}_1^r\rangle|\right)}. \tag{6}$$

Reference [1] also introduces the static quasicurrent $\dot{\mathbb{Q}}_1 = \dot{Q}_1 + \dot{W}_1$. According to (4), we have

$$\dot{\mathbb{Q}}_1 = \frac{dE_1}{dt} + \frac{1}{2}C_0(X_1 - X_2)\left(\frac{dX_1}{dt} + \frac{dX_2}{dt}\right), \tag{7}$$

so that, when we take the time and statistical averages after a steady state has been established in the system, i.e., $\langle dE_1/dt\rangle = 0$, we simply get

$$\langle\dot{\mathbb{Q}}_1\rangle = \left\langle\frac{1}{2}C_0(X_1 - X_2)\left(\frac{dX_1}{dt} + \frac{dX_2}{dt}\right)\right\rangle. \tag{8}$$

In this two-oscillator system, $\langle\dot{\mathbb{Q}}_1\rangle$ has a simple interpretation in terms of the power J flowing through the coupling link C_0. The force F_1 exerted on particle 1 due to the coupling is $F_1 = -C_0(X_1 - X_2)$ and therefore the power $\mathcal{P}_1$ transmitted *to* particle 1 due to the coupling is $\mathcal{P}_1 = F_1\frac{dX_1}{dt} = -C_0(X_1 - X_2)\frac{dX_1}{dt}$. Similarly, the force F_2 due to the coupling is $F_2 = C_0(X_1 - X_2)$ and the power transmitted *to* particle 2 is $\mathcal{P}_2 = F_2\frac{dX_2}{dt} = C_0(X_1 - X_2)\frac{dX_2}{dt}$. Therefore the average power transfer *from* particle 1 *to* particle 2 is

$$\langle J\rangle = -\langle\mathcal{P}_1\rangle + \langle\mathcal{P}_2\rangle$$
$$= \left\langle C_0(X_1 - X_2)\left(\frac{dX_1}{dt} + \frac{dX_2}{dt}\right)\right\rangle = 2\langle\dot{\mathbb{Q}}_1\rangle. \tag{9}$$

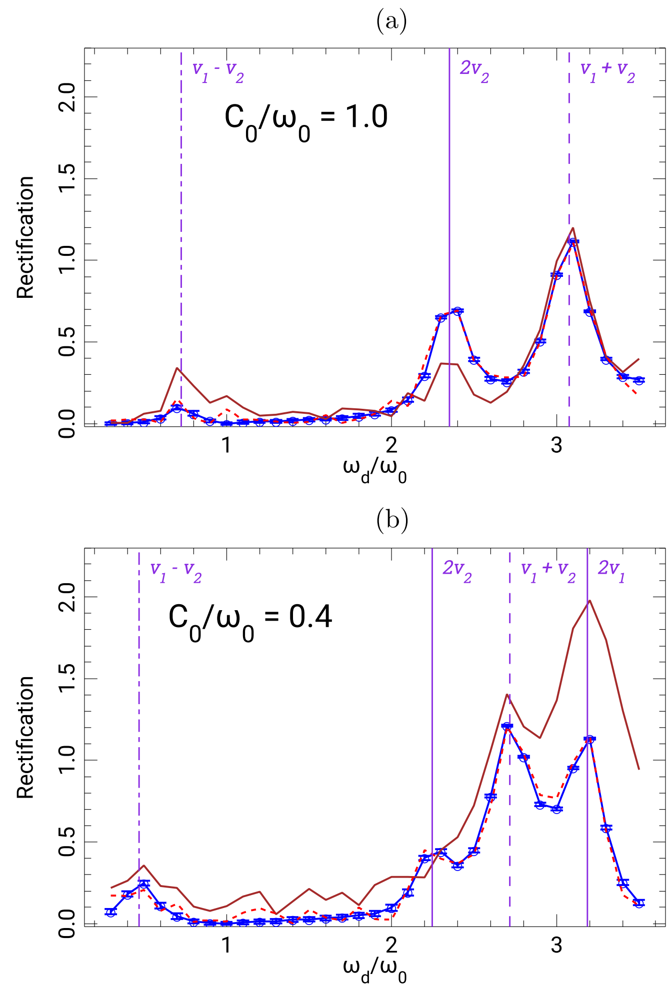

FIG. 2. Rectification coefficients versus the modulation frequency ω_d for two values of the coupling constant C_0: (a) $C_0/\omega_0 = 1.0$ and (b) $C_0/\omega_0 = 0.4$. Brown full line, R_Q; blue full line with error bars, R_J; red dashed line, $R_{\mathbb{Q}}$. The vertical lines show some of the combination of the eigenfrequencies ν_1/ω_0, ν_2/ω_0 of the system of two oscillators.

Therefore the rectification coefficient of Ref. [1] defined in terms of the static quasicurrents

$$R_{\mathbb{Q}} = \frac{|\langle\dot{\mathbb{Q}}_1\rangle + \langle\dot{\mathbb{Q}}_1^r\rangle|}{\max\left(|\langle\dot{\mathbb{Q}}_1\rangle|, |\langle\dot{\mathbb{Q}}_1^r\rangle|\right)} \tag{10}$$

should coincide with the rectification coefficient R_J defined from the calculations of the fluxes $\langle J\rangle$ and $\langle J^r\rangle$ in the simulations

$$R_J = \frac{|\langle J\rangle + \langle J^r\rangle|}{\max(|\langle J\rangle|, |\langle J^r\rangle|)}. \tag{11}$$

Figure 2 shows the rectification coefficients R_Q, R_J, and $R_{\mathbb{Q}}$ versus the driving frequency ω_d for two values of the coupling coefficient C_0. The calculations have been made with $\gamma = 0.1$

for the Langevin equation, i.e., a moderate strength of the coupling with the thermostats. Decreasing γ makes the peaks sharper. The horizontal scale for ω_d/ω_0 is the same as on Fig. 3 of Ref. [1] to allow an easier comparison. The coefficients R_Q and $R_{\mathbb{Q}}$, which involve the evaluation of the heat fluxes from the thermostats, show fluctuations which result from an averaging over 200 realizations only. Their error bars are not shown to preserve the readability of the figure, but they are significantly larger than the error bars on R_J. Nevertheless, the equality between R_J and $R_{\mathbb{Q}}$ shows up clearly, giving a direct meaning to the rectification defined in terms of the static quasicurrents by showing that, as expected, it is due to the transfer along the coupling link.

The analogies with the results of Ref. [1] are clear. In particular, as in the quantum case, the regions with nonzero rectification correspond to a driving at combinations of the eigenfrequencies of the system. There are nevertheless some differences between the classical and quantum cases. In Ref. [1], the authors point out that the rectification coefficient $R_{\mathbb{Q}}$ computed with the quasistatic heat currents does not show the regions of high rectification corresponding to $\omega_d = 2\nu_1, 2\nu_2$ which are detected with R_Q derived from the fluxes $\dot{Q}_1$ and $\dot{Q}_1^r$. They analyze this in terms of normal mode interactions. In the classical case, we do find that $R_{\mathbb{Q}}$ is significantly lower than R_Q for $\omega_d = 2\nu_1$ [Fig. 2(b)], but it does not fully vanish, and we do not find a similar effect for $\omega_d = 2\nu_2$. This suggests that the effect of the classical heat bath on mode interactions is not the same as in the quantum case. Moreover, we can also expect different laws for the temperature dependence of the rectification effect when the system obeys classical or quantum statistics.

Although there are some differences between the classical and quantum cases, the results show that the concept of dynamically induced heat rectification, introduced in Ref. [1] is not confined to the quantum case and is instead a phenomenon of general validity. Therefore its understanding should not be specifically sought in quantum effects but in general features of the system. In the classical case the mechanism that leads to the rectification may be related to a kind of parametric resonance because the calculation of $\dot{W}_1$ also exhibits large peaks at combinations of the eigenfrequencies of the system of coupled oscillators.

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[5] The caption of Fig. 3 of Ref. [1] indicates $\omega_1 = 2\omega_0$; however, the curves plotting the eigenfrequencies of the two-oscillator system correspond to $\omega_1^2 = 2\omega_0^2$.

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