Quantum thermal diode based on two interacting spinlike systems under different excitations

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We demonstrate that two interacting spinlike systems characterized by different excitation frequencies and coupled to a thermal bath each, can be used as a quantum thermal diode capable of efficiently rectifying the heat current. This is done by deriving analytical expressions for both the heat current and rectification factor of the diode, based on the solution of a master equation for the density matrix. Higher rectification factors are obtained for lower heat currents, whose magnitude takes their maximum values for a given interaction coupling proportional to the temperature of the hotter thermal bath. It is shown that the rectification ability of the diode increases with the excitation frequencies difference, which drives the asymmetry of the heat current, when the temperatures of the thermal baths are inverted. Furthermore, explicit conditions for the optimization of the rectification factor and heat current are explicitly found.

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I. INTRODUCTION

Guiding, rectification, and amplification of electrical and thermal currents are of critical importance to efficiently manage the energy resources of nature. In electricity, this has been done with diodes [1] and transistors [2], which have revolutionized our daily life. Thermal analogs of these fundamental electronic devices making possible the heat current control do not exist yet, despite the fact that around 60% of the energy used in the worldwide industry is lost as waste heat. Harvesting and managing this energy is thus a huge scientific challenge nowadays due to limited energy resources, high economic expenses, and global warming issues.

Inspired by the capabilities of the electronic diode and transistor, researchers conceived the thermal diode [3,4] and thermal transistor [5–8] by heat conduction [9–15] and heat radiation [16–22]. The theoretical predictions of these conceptions for switching on and off the heat current were experimentally observed in carbon nanotube structures [23], semiconductor quantum dots [24], oxide materials [25], and vanadium dioxide (VO_2) [26,27], which has recently attracted a lot of interest due to its dielectric-to-metal transition at temperatures near room temperature [28]. The heat current can be enhanced with VO_2 in its dielectric phase and cut down when it becomes metallic [29], which results in a thermal diode with a rectification factor close to unity [7,30,31], and a radiative thermal transistor with amplification factors higher than 10 [6,8].

Quantum systems, such as atoms and quantum dots have been used to develop photonic rectifiers [32–34] and optical [35], electromagnetic [36], and thermal [37] transistors. The heat transport through a system of two strongly interacting sites coupled to two and three thermal baths has also been analyzed by Werlang [38,39] and Man *et al.* [40], respectively. In these three latter works, authors reported fine control of the heat currents and their asymmetry driving the thermal rectification. However, they did not put so much attention on the rectification optimization by means of the difference of excitation frequencies applied to each quantum site, which is considered in the present work.

The objective of this paper is to theoretically demonstrate that two interacting spinlike systems characterized by different excitation frequencies and coupled to a thermal bath each, can be used as an efficient quantum thermal diode. This is done by deriving analytical expressions for both the heat current and rectification factor of the diode, and exploiting the asymmetry introduced by the difference of excitation frequencies on the heat current. We show that the heat current saturates as the temperature difference between the thermal baths increases and that its magnitude reaches a maximum value for a critical coupling strength.

II. THEORETICAL MODELING

Let us consider a quantum thermal diode made up of two interacting spinlike systems characterized by the excitation frequencies ω_L and ω_R, and coupled to thermal baths set at temperatures T_L and T_R, as shown in Fig. 1. These frequencies may be smaller or greater than the coupling strength Δ and can be associated, for instance, to magnetic fields applied along the z direction. The heat currents J_L and J_R exchanged by the thermal baths are, therefore, determined not only by $T_L \neq T_R$, but also by ω_L, ω_R, and Δ, which drive the thermal rectification of the diode, as shown below. The behavior of this diode is governed by the Hamiltonian

$$H = \frac{\hbar}{2}\left(\omega_L \sigma_z^L + \omega_R \sigma_z^R + \Delta \sigma_z^L \sigma_z^R\right), \tag{1}$$

where $2\pi\hbar$ is the Planck constant and σ_z^n is the Pauli matrix z with eigenstates $|+\rangle$ (spin up) and $|-\rangle$ (spin down), for the system $n = L; R$. In terms of these individual eigenstates, the four ones of H are labeled as $|1\rangle = |++\rangle$, $|2\rangle = |+-\rangle$, $|3\rangle = |-+\rangle$, and $|4\rangle = |--\rangle$. The allowed energy transitions of the system are determined by the frequencies $\omega_{ij} = (\epsilon_i - \epsilon_j)/\hbar > 0$, where ϵ_m is the eigenvalue of H for the eigenstate $|m\rangle$. Equation (1) establishes that $\omega_{12} = \omega_R + \Delta$, $\omega_{13} = \omega_L + \Delta$, $\omega_{14} = \omega_L + \omega_R$, $\omega_{23} = \omega_L - \omega_R$, $\omega_{24} = \omega_L - \Delta$, and $\omega_{34} = \omega_R - \Delta$.

The interaction between the spinlike systems and their respective thermal baths constituted of harmonic oscillators is described by the spin-boson model in the x component,

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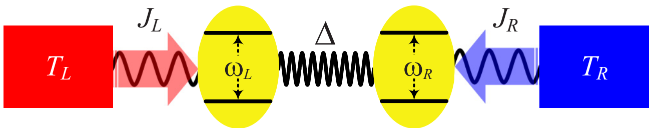

FIG. 1. Scheme of a quantum thermal diode made up of two interacting spinlike systems connected to thermal baths at temperatures T_L and T_R.

through the following Hamiltonian [38]

$$H^n_{\text{spin-bath}} = \sigma^n_x \sum_k g_k \left(a^n_k + a^{n\dagger}_k\right), \tag{2}$$

where g_k is the coupling strength of both thermal baths and $a^{n\dagger}_k$ (a^n_k) is the creation (annihilation) operator describing the boson mode k of the bath $n = L; R$, whose Hamiltonian is $H^n_{\text{bath}} = \sum_k \omega_k a^{n\dagger}_k a^n_k$. Equation (2) establishes that the left (right) bath only induces transitions on the left (right) spinlike system, so the transitions $|1\rangle \leftrightarrow |3\rangle$ and $|2\rangle \leftrightarrow |4\rangle$ are induced by the left bath, while the ones $|1\rangle \leftrightarrow |2\rangle$ and $|3\rangle \leftrightarrow |4\rangle$ are driven by the right bath. Furthermore, the transitions $|1\rangle \leftrightarrow |4\rangle$ and $|2\rangle \leftrightarrow |3\rangle$, which simultaneously flip both spins, are forbidden.

The heat current J_n that the thermal bath n introduces into the system is given by [39,41]

$$J_n = \text{Tr}(\mathcal{L}_n[\rho]H), \tag{3}$$

where ρ is the density matrix with unity trace [$\text{Tr}(\rho) = 1$] and the Lindblad operator $\mathcal{L}_n[\rho]$ is defined by [42]

$$\mathcal{L}_n[\rho] = \sum_{\omega>0} \mathcal{I}(\omega)[(1 + f_n(\omega))B_n(\omega) + f_n(\omega)C_n(\omega)], \tag{4a}$$

$$B_n(\omega) = A_n(\omega)\rho A^\dagger_n(\omega) - \frac{1}{2}\{\rho, A^\dagger_n(\omega)A_n(\omega)\}, \tag{4b}$$

$$C_n(\omega) = A^\dagger_n(\omega)\rho A_n(\omega) - \frac{1}{2}\{\rho, A_n(\omega)A^\dagger_n(\omega)\}, \tag{4c}$$

$$A_n(\omega) = \sum_{\omega>0} |j\rangle\langle j|\sigma^n_x|i\rangle\langle i|, \tag{4d}$$

$$f_n(\omega) = \frac{1}{e^{\hbar\omega/(k_B T_n)} - 1}, \tag{4e}$$

for all transition frequencies $\omega \equiv \omega_{ij} > 0$. We assume that the thermal baths are ohmic, such that the spectral function $\mathcal{I}(\omega) = k\omega$, k being a dimensionless constant. Considering first that $\Delta < \omega_L; \omega_R$ and taking into account that the Pauli matrix σ^n_x satisfies the relation $\sigma^n_x|\pm\rangle = |\mp\rangle$, Eq. (4d) establishes that the only nonvanishing operators $A_n(\omega)$ are $A_L(\omega_{13}) = |3\rangle\langle 1|$ and $A_L(\omega_{24}) = |4\rangle\langle 2|$ for $\mathcal{L}_L[\rho]$, and $A_R(\omega_{12}) = |2\rangle\langle 1|$ and $A_R(\omega_{34}) = |4\rangle\langle 3|$ for $\mathcal{L}_R[\rho]$. After inserting these results in Eqs. (4a) to (4c), one obtains

$$\mathcal{L}_L[\rho] = \Gamma^L_{13}(|3\rangle\langle 3| - |1\rangle\langle 1|) + \Gamma^L_{24}(|4\rangle\langle 4| - |2\rangle\langle 2|), \tag{5a}$$

$$\mathcal{L}_R[\rho] = \Gamma^R_{12}(|2\rangle\langle 2| - |1\rangle\langle 1|) + \Gamma^R_{34}(|4\rangle\langle 4| - |3\rangle\langle 3|), \tag{5b}$$

where the net decay rate Γ^n_{ij} from the state $|i\rangle$ to $|j\rangle$ is defined by

$$\Gamma^n_{ij} = k\omega_{ij}[(1 + f_n(\omega_{ij}))\rho_{ii} - f_n(\omega_{ij})\rho_{jj}], \tag{6}$$

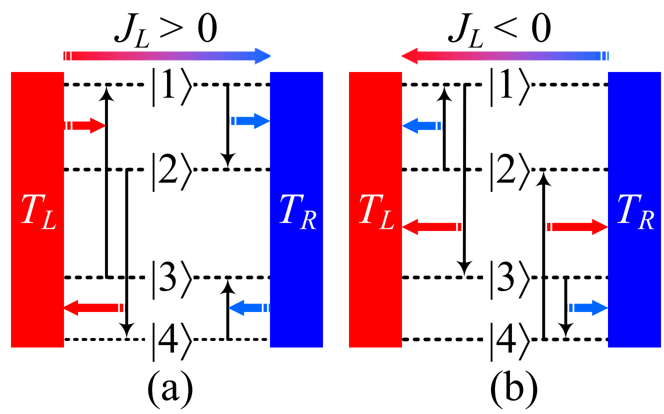

FIG. 2. Energy transitions allowing the flow of heat current from (a) the left bath to the right one ($\Gamma < 0$) and (b) the other way around ($\Gamma > 0$). The colored thick arrows stand for the direction of the heat current associated to each transition.

ρ_{mm} being the diagonal elements of the density matrix ρ, which for the steady-state regime of heat conduction considered in this work obeys the master equation [38]

$$\mathcal{L}_L[\rho] + \mathcal{L}_R[\rho] = 0, \tag{7}$$

where we have neglected the contribution of the counter rotating terms due to their rapid oscillation behavior, as was demonstrated by Breuer and Petruccione [43]. Taking into account that $\Gamma^n_{ij} = -\Gamma^n_{ji}$, the combination of Eqs. (5) and (7) yields

$$\Gamma^L_{13} = \Gamma^R_{21} = \Gamma^L_{42} = \Gamma^R_{34} \equiv \Gamma, \tag{8}$$

which indicates that the involved transitions have the same decay rate Γ, determined by the parameters ω_n, T_n, and Δ. According to Eqs. (3) and (5), the heat currents J_n are

$$J_L = -\hbar\omega_{13}\Gamma^L_{13} + \hbar\omega_{24}\Gamma^L_{42} = -2\hbar\Delta\Gamma, \tag{9a}$$

$$J_R = \hbar\omega_{12}\Gamma^R_{21} - \hbar\omega_{34}\Gamma^R_{34} = 2\hbar\Delta\Gamma, \tag{9b}$$

which show that $J_L + J_R = 0$, as established by the principle of energy conservation. Note that the heat current flows from the left bath to the right one through the interacting spinlike systems, when $J_L > 0$ ($\Gamma < 0$). Equation (9a) indicates that the left thermal bath absorbs (delivers) from (to) the left spinlike system the energy $\hbar\omega_{13}$ ($\hbar\omega_{24}$) at the rate $|\Gamma|$, resulting in the net exchanged energy of $2\hbar\Delta$. The graphical representation of Eqs. (9a) and (9b) is shown in Figs. 2(a) and 2(b), for $\Gamma < 0$ and $\Gamma > 0$, respectively. In both cases, the transition between the states $|2\rangle$ and $|4\rangle$ generates a heat current opposite to the net one J_L and therefore it is expected to drive the rectification of J_L.

The system of Eqs. (8) along with the condition $\text{Tr}(\rho) = 1$ can conveniently be solved for Γ by expressing the Bose-Einstein distribution function as $f_n(\omega) = 0.5\exp(-\alpha_n\omega/2)/\sinh(\alpha_n\omega/2)$, where $\alpha_n = \hbar/(k_B T_n)$. The final result for J_L is

$$J_L = \frac{k\hbar\Delta}{D}\left(\omega^2_L - \Delta^2\right)\left(\omega^2_R - \Delta^2\right)\sinh[(\alpha_R - \alpha_L)\Delta], \tag{10}$$

where

$$D = \omega_R(\omega_L^2 - \Delta^2)C + \omega_L(\omega_R^2 - \Delta^2)B + \Delta\{(2\Delta^2 - \omega_L^2 - \omega_R^2)A + (\omega_R^2 - \omega_L^2)\sinh[(\alpha_R - \alpha_L)\Delta]\}, \tag{11a}$$

$$C = [\cosh(\alpha_L\omega_L) + \cosh(\alpha_L\Delta)]\sinh(\alpha_R\omega_R) + \sinh(\alpha_L\omega_L)\sinh(\alpha_R\Delta), \tag{11b}$$

$$B = [\cosh(\alpha_R\omega_R) + \cosh(\alpha_R\Delta)]\sinh(\alpha_L\omega_L) + \sinh(\alpha_R\omega_R)\sinh(\alpha_L\Delta), \tag{11c}$$

$$A = \sinh(\alpha_L\omega_L)\sinh(\alpha_R\omega_R) + \cosh(\alpha_R\omega_R)\sinh(\alpha_L\Delta) + \cosh(\alpha_L\omega_L)\sinh(\alpha_R\Delta). \tag{11d}$$

Even though Eqs. (10) and (11) have been derived for $\Delta < \omega_L;\omega_R$, they still hold for $\Delta > \omega_L$ and/or $\Delta > \omega_R$. This can be shown by redoing the above-developed calculations with $\omega_{42} = \Delta - \omega_L > 0$ and/or $\omega_{43} = \Delta - \omega_R > 0$, and using the fact that the decay rate $\Gamma_{ij}^n = -\Gamma_{ji}^n$. In doing so, the ultimate result $J_L = -J_R = -2\hbar\Delta\Gamma$ in Eqs. (9a) and (9b) remains valid as well. The following general features of Eqs. (10) and (11) are worth mentioning: (1) The denominator $D(\alpha_L,\alpha_R,\omega_L,\omega_R,\Delta) = D(\alpha_R,\alpha_L,\omega_R,\omega_L,\Delta)$ is invariant under an interchange of temperatures and excitation frequencies, while the heat current $J_L(\alpha_L,\alpha_R,\omega_L,\omega_R,\Delta) = -J_L(\alpha_R,\alpha_L,\omega_R,\omega_L,\Delta)$ changes sign only, as expected. (2) Irrespective of the particular values of T_L and T_R, $D > 0$ for $\Delta < \omega_L;\omega_R$ or $\Delta > \omega_L;\omega_R$, which indicates that the heat current $J_L > 0$ ($J_L < 0$) flows from the left (right) bath to the right (left) one, for $T_L > T_R$ ($T_L < T_R$), as established by the second law of thermodynamics. It is thus clear that the direction of the heat current is only determined by the sign of the temperature difference $T_L - T_R$ and not by the relative values of Δ with respect to ω_L and ω_R. (3) The heat current vanishes ($J_L = 0$), for $\Delta = 0;\infty$ or $\omega_L;\omega_R = \infty$. This shows that there exists a critical coupling strength Δ for which J_L is maximum, provided that the excitation frequencies ω_L and ω_R remain finite, as is the case of practical interest. The numerical values of this critical Δ are found and analyzed in Sec. III. (4) In the classical regime of high temperature and weak coupling, such that $\alpha_n\Delta \ll \alpha_n\omega_n \ll 1$, Eq. (10) reduces to $J_L = k\hbar\Delta^2(T_L - T_R)/(T_L + T_R)$, which is consistent with the macroscopic Fourier law of heat conduction. (5) The difference between the magnitudes of $J_L(\alpha_L,\alpha_R,\omega_L,\omega_R,\Delta)$ and $J_L(\alpha_R,\alpha_L,\omega_L,\omega_R,\Delta)$ is determined by the ratio ω_R/ω_L (or difference $\omega_L - \omega_R$) of excitation frequencies, such that it vanishes for $\omega_R = \omega_L$. This points out that the modulation of the external frequencies ω_L and ω_R through different values provides the possibility of allowing the flow of heat current in one direction (switch on) and blocking it in the opposite one (switch off). The effectiveness of the quantum thermal diode to generate this thermal rectification can be properly quantified by means of the rectification factor R defined as follows [8,44]:

$$R = \frac{|J_L(\alpha_L,\alpha_R) + J_L(\alpha_R,\alpha_L)|}{\mathrm{Max}(|J_L(\alpha_L,\alpha_R)|,|J_L(\alpha_R,\alpha_L)|)}, \tag{12}$$

where, by briefness, the dependence of J_L on ω_L, ω_R, and Δ is not written, but understood. The quantum thermal diode could, therefore, exhibit near perfect rectification ($R = 1$), when one of the involved heat currents is much larger than the other one. After inserting Eq. (10) into Eq. (12), R takes the form

$$R = 1 - \frac{D(\alpha_L,\alpha_R,\omega_L,\omega_R,\Delta)}{D(\alpha_R,\alpha_L,\omega_L,\omega_R,\Delta)}, \tag{13}$$

which reduces to $R = 0$, for $\omega_L = \omega_R$, as expected. Equation (13) has been derived assuming that its numerator is smaller than its denominator and, if this is not the case, they should be interchanged. In any case, Eq. (13) indicates that the rectification of the heat current is totally determined by its denominator defined in Eq. (11a). To better understand the behavior of J_L and R, we are going to consider the following limiting cases:

A. High temperature bath: $\theta_L \gg \max(1,a,\theta_R)$

In this case, the left (right) thermal bath is at high (low) normalized temperature $\theta_n = k_B T_n/(\hbar\omega_L)$, and Eqs. (10) and (13) reduce to

$$\frac{J_L}{J_0} = \frac{a(a^2 - b^2)\sinh(a/\theta_R)}{a\sinh(a/\theta_R) - b\sinh(b/\theta_R)}, \tag{14a}$$

$$R = 1 - \begin{cases} \chi, & b < 1 \\ \frac{1}{\chi}, & b > 1, \end{cases} \tag{14b}$$

$$\chi = \frac{a^2 - 1}{a^2 - b^2}\,\frac{a\sinh(a/\theta_R) - b\sinh(b/\theta_R)}{a\sinh(a/\theta_R) - \sinh(1/\theta_R)}, \tag{14c}$$

where $a = \Delta/\omega_L$, $b = \omega_R/\omega_L$, and $J_0 = k\hbar\omega_L^2/2$. Note that both J_L and R vanish, when the frequency ratio $b \gg \max(1,\theta_R)$, which indicates that the excitation frequency of the spinlike system coupled to the hotter thermal bath should not be so high with respect to that of the other system. For $\theta_R \gg \max(a,b)$, Eq. (14a) reduces to $J_L = J_0 a^2 = k\hbar\Delta^2/2$, which represents the heat current of saturation reached by the system when its thermal baths are set at high temperatures, such that $T_L \gg T_R \gg T_0\max(1,a)$, with $T_0 = \hbar\omega_L/k_B$. Under this latter temperature regime and the additional condition $\theta_R \gg b$, Eqs. (14b) and (14c) become

$$R = \begin{cases} \frac{1-b^2}{6\theta_R^2+a^2+1}, & b < 1 \\ \frac{b^2-1}{6\theta_R^2+a^2+b^2}, & b > 1, \end{cases} \tag{15}$$

which shows that the rectification decreases with the inverse of θ_R^2 mainly, and takes its maximum value for $b = 0$ ($\omega_R = 0$). On the other hand, for $\theta_R \ll \min(a,b)$, $J_L = 0$ [$J_L = J_0(a^2 - b^2)$] when $b > a$ ($b < a$). It is, therefore, clear that after fixing the bath temperatures $T_L \gg T_0\max(1,a) \gg T_R$, the heat current can be switched on and switched off by modulating the applied excitation frequency ω_R through values smaller ($\omega_R < \Delta$) and larger ($\omega_R > \Delta$) than the coupling strength, respectively. This latter result shows that the heat current can not only be rectified with the temperature, as defined in Eq. (12), but also with the modulation of ω_R.

B. Asymmetrical excitation: $\omega_L > \omega_R = 0$

In this case, Eq. (9) reduces to

$$\frac{J_L}{J_0} = \frac{2a^2(1-a^2)\sinh[(1/\theta_R - 1/\theta_L)a]}{(1-2a^2)A_0 + \sinh[(1/\theta_R - 1/\theta_L)a] + aB_0}, \tag{16a}$$

$$A_0 = \sinh(a/\theta_L) + \cosh(1/\theta_L)\sinh(a/\theta_R), \tag{16b}$$

$$B_0 = [1+\cosh(a/\theta_R)]\sinh(1/\theta_L). \tag{16c}$$

Equation (16a) coincides with the result derived by Werlang *et al.* [38] for $\Delta < \omega_L$, and here we have shown that it is also valid for $\Delta > \omega_L$. For $\theta_L \gg \max(1,a,\theta_R)$, Eq. (16a) reduces to Eq. (14a), with $b = 0$, as expected. On the other hand, when $\theta_L \ll \min(1,a,\theta_R)$, the heat current takes the form

$$\frac{J_L}{J_0} = \begin{cases} 0, & a < 1 \\ \frac{-a(a^2-1)e^{-a/\theta_R}}{a\cosh(1/\theta_R) - \sinh(1/\theta_R)}, & a > 1. \end{cases} \tag{17}$$

As in the case of Eq. (14a), Eq. (17) shows that J_L can be switched on and switched off by modulating the relative coupling strength $a = \Delta/\omega_L$. For $a > 1$, the maximum (saturation) heat current from the right bath to the left one is $J_L = -J_0(a^2-1)$, which can be reached by rising the temperature of the right bath, such that $T_R \gg aT_0 > T_0 \gg T_L$.

C. Weak Coupling: $\Delta \ll \min(\omega_L,\omega_R)$

In this case of relatively weak interaction between the two spinlike systems, the heat current in Eq. (10) becomes

$$J_L = \frac{k(\hbar\Delta)^2}{k_B}\frac{\omega_L\omega_R(1/T_R - 1/T_L)}{\omega_L\chi_{LR} + \omega_R\chi_{RL}}, \tag{18}$$

where $\chi_{nm} = [1+\cosh(\alpha_n\omega_n)]\sinh(\alpha_m\omega_m)$. The symmetric Eq. (18) makes explicit the general fact that $J_L > 0$ ($J_L < 0$) for $T_L > T_R$ ($T_L < T_R$), and shows that the heat current increases with the square of the coupling strength ($J_L \propto \Delta^2$). For $T_L \gg T_0$, the heat current along with the corresponding rectification factor [see Eq. (13)] driven by the denominator of Eq. (18) are given by

$$J_L = \frac{k\hbar\Delta^2}{2}\frac{b/\theta_R}{\sinh(b/\theta_R)}, \tag{19a}$$

$$R = 1 - \begin{cases} \frac{\sinh(b/\theta_R)}{b\sinh(1/\theta_R)}, & b < 1 \\ \frac{b\sinh(1/\theta_R)}{\sinh(b/\theta_R)}, & b > 1. \end{cases} \tag{19b}$$

Note that as the normalized temperature $\theta_R = T_R/T_0$ of the right thermal bath increases through values greater than unity, the rectification factor tends to vanish, while the heat current goes to its maximum value $J_L = k\hbar\Delta^2/2$. On the other hand, for $\theta_R \ll \min(1,b)$, $J_L = 0$, and $R = 1$ ($R = 0$) for $b < 1$ ($b > 1$). This tradeoff between J_L and R holds not only for weak couplings, but also for strong ones, as shown in Sec. III. By analogy to the optical diode [33,34,45], this tradeoff could be optimized through a sort of thermal diode efficiency η defined as $\eta = R\tau$, where $\tau = |J_L(\alpha_L,\alpha_R)|/|J_L(\alpha_L,\alpha_R) + J_L(\alpha_R,\alpha_L)|$ is the transport efficiency from the left bath to the right one. Based on the definition of the rectification factor R in Eq. (12), one finds $\eta = 1 - R$, which indicates that, in our formalism, η is nothing more than the complement of R and therefore

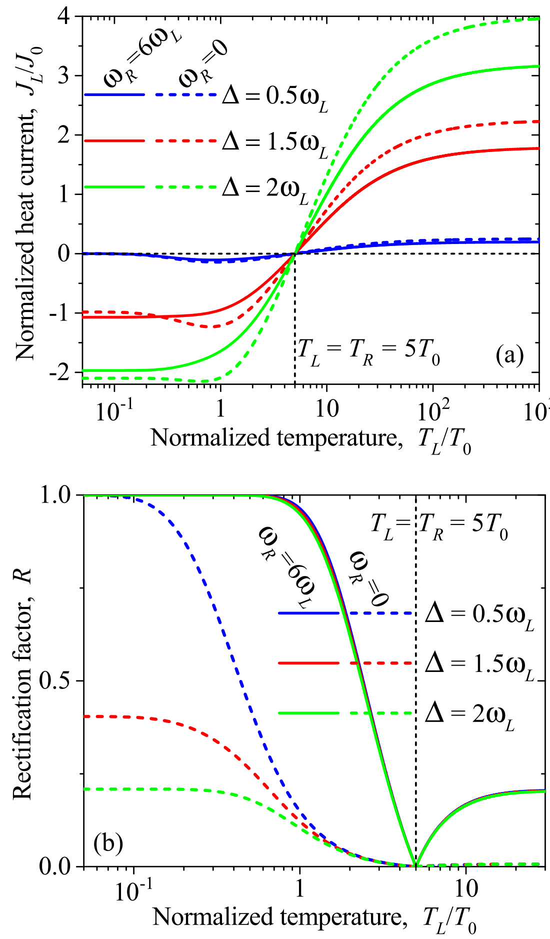

FIG. 3. (a) Normalized heat current and (b) rectification factor as functions of the normalized temperature of the left bath. Calculations are done using $T_0 = \hbar\omega_L/k_B$ and $J_0 = k\hbar\omega_L^2/2$.

can be associated to the behavior of the heat current. In our formalism, the rectification factor represents a rectification efficiency that takes the value of $R = 0$ ($R = 1$) in absence of (presence of perfect) rectification. However, the thermal diode ability of rectifying the heat current can also be defined in other alternative ways [34], for which η is not necessarily the complement of R. Taking into account that J_L can be enhanced through the parameter k of the spectral function, without affecting the values of R, our primary interest in this work is the optimization of R, using its common definition in Eq. (12) [4,7,8,40,44].

III. RESULTS AND DISCUSSION

The heat current J_L and rectification factor R of the quantum thermal diode shown in Fig. 1, are now analyzed for weak ($\Delta < \omega_n$) and strong ($\Delta > \omega_n$) interactions between its spinlike systems.

Figures 3(a) and 3(b) show the behavior of the heat current and rectification factor as functions of the normalized temperature T_L/T_0 of the left bath. Note that $J_L > 0$ ($J_L < 0$) flows from the left (right) bath to the right (left) one, when $T_L > T_R$ ($T_L < T_R$), such that it saturates for high (low) enough T_L/T_0. This saturation in the energy flux is due to

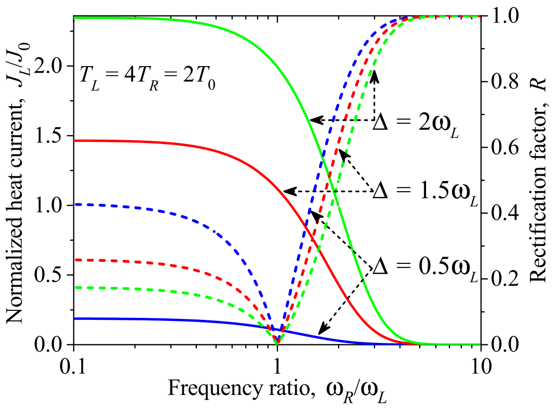

FIG. 4. Normalized heat current and rectification factor as functions of the ratio ω_R/ω_L of excitation frequencies. The solid and dashed lines stand for the heat current and rectification factor, respectively.

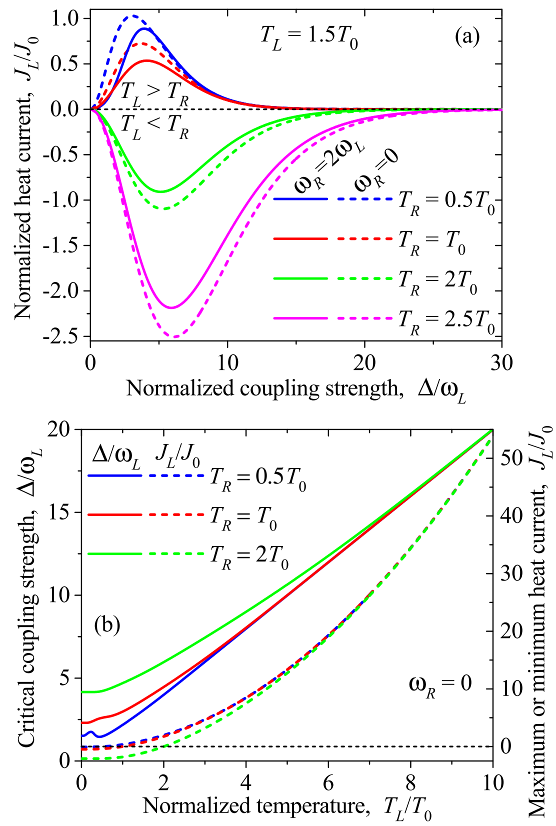

FIG. 5. (a) Heat current and (b) critical coupling strength as functions of the normalized coupling strength and normalized temperature of the left bath, respectively. The solid and dashed lines in (b) stand for the critical coupling and maximum or minimum heat current, respectively. Calculations are done for $\omega_R = 0$.

the limited number of energy levels (Fig. 2), and its values for $T_L/T_0 \gg 1$ are given by Eq. (14a). Higher saturation currents are obtained for stronger coupling strengths Δ and a lower excitation frequency ω_R of the spinlike system connected to the cold thermal bath. This indicates that Δ (ω_R) acts like a thermal conductance (resistance), for the flow of heat current through the quantum thermal diode. For $\Delta = 0.5\omega_L$, the low-temperature current vanishes, while the high-temperature one is finite. According to Eq. (10), this behavior holds for any $\Delta < \omega_L$, as long as $\omega_R = 0$. This relatively strong asymmetry of J_L with respect to that for $\Delta > \omega_L$ is responsible for its higher rectification tending to unity for $\omega_R = 0$ and the low-temperature regime, as shown in Fig. 3(b). Under these conditions, Figs. 3(a) and 3(b) show that higher heat currents are associated with lower rectifications and vice versa. For $\omega_R = 6\omega_L$, on the other hand, R becomes almost independent of $a = \Delta/\omega_L$ and is higher than the corresponding one for $\omega_R = 0$. In the high-temperature regime, the rectification factor tends to $R \approx 18\%$, which can be enhanced by increasing the ratio $b = \omega_R/\omega_L$ and/or reducing a and $\theta_R = T_R/T_0$, as established by Eq. (15). It is thus clear that the regime of $\omega_R/\omega_L > 1$ generally yields higher rectification than the one of $\omega_R/\omega_L = 0$, for both the low- and high-temperature regimes of the left thermal bath. This is confirmed by Fig. 4, which shows that the frequency regime $\omega_R/\omega_L > 1$ is better than the one set by $\omega_R/\omega_L < 1$ for enhancing the rectification factor to values near unity. This optimization of R by increasing $\omega_R/\omega_L > 1$ can only be achieved with low heat currents, and hence this frequency ratio should be chosen high enough to enhance R, but low enough to not reduce so much the heat current with respect to J_0.

The normalized heat current J_L/J_0 as a function of the normalized coupling strength Δ/ω_L is shown in Fig. 5(a). As one can see, J_L vanishes in the absence of coupling ($\Delta = 0$) and in the presence of an ultrastrong one ($\Delta/\omega_L \gg 1$). This latter fact arises because, in this limit, the decay rate from the state $|i\rangle$ to $|j\rangle$ becomes equal to the excitation rate from $|j\rangle$ to $|i\rangle$, which yields a net decay rate $\Gamma_{ij} = 0$. The magnitude of the maximum (minimum) heat current obtained for $T_L > T_R$ ($T_L < T_R$) decreases as the ratio ω_R/ω_L increases, and it occurs at the critical coupling strength shown in Fig. 5(b) for $\omega_R = 0$. As the left bath temperature increases through values $T_L \gg T_0$, this critical coupling becomes independent of the right bath temperature and varies linearly with T_L/T_0, through the simple relation $\Delta/\omega_L = 2T_L/T_0$. In general, the maximum or minimum of the heat current appears for $\Delta/\omega_L > 1$ and is nearly independent of T_R/T_0, as shown by the dashed lines in Fig. 5(b). Hence, one straight way to maximize the magnitude of the heat current is by setting the thermal bath temperatures, excitation frequencies, and coupling strength, such that they fulfill the "key rule" $\Delta/\omega_L = 2T_L/T_0 \gg \max(1, 2T_R/T_0)$ and $\omega_R = 0$.

Figure 6(a) shows the characteristic curve $J_L(\delta T)$ of the quantum thermal diode for a constant average temperature $T = (T_L + T_R)/2 = 1.5T_0$. When $\omega_R = 0$, the magnitude of the heat current is generally higher than the corresponding one for $\omega_R = 2\omega_L$, which introduces a strong asymmetry on the values of J_L around $\delta T = T_L - T_R = 0$. This asymmetry of J_L increases with the frequency ratio ω_R/ω_L and temperature difference $|\delta T|$, and disappears when $|\delta T| \ll T_0$, for which the heat current exhibits a linear behavior. This indicates that the rectification factor R also increases with ω_R/ω_L and $|\delta T|$, as shown in Fig. 6(b). In contrast to J_L, higher rectification is obtained for lower coupling strength, which is consistent with Figs. 3(a) and 3(b). For $\omega_R = 2\omega_L$, the maximum (saturation) values of R are higher than the corresponding

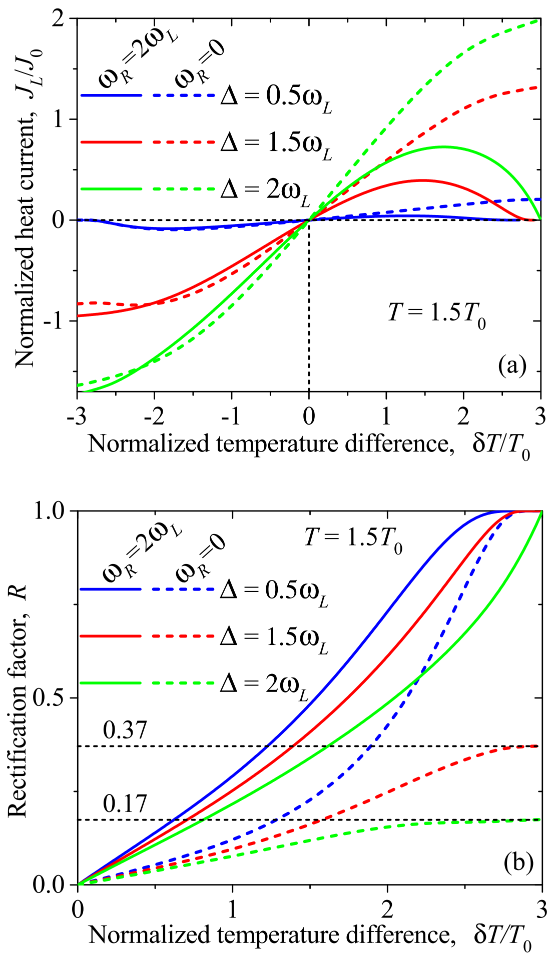

FIG. 6. (a) Normalized heat current and (b) rectification factor as functions of the normalized temperature difference $\delta T/T_0 = (T_L - T_R)/T_0$. Calculations are done for $T = (T_L + T_R)/2 = 1.5T_0$.

ones for $\omega_R = 0$, as established by Eq. (15), and they are reached at $\delta T = 2T(T_L \gg T_R$ or $T_R = 0)$. It is clear that, based on Figs. 3(b), 4, and 6(b), the rectification can be better optimized with an excitation frequency $\omega_R > \omega_L$, rather than with $\omega_R = 0$, provided that $T_L > T_R$.

Given that the R (J_L) is independent of (proportional to) the dimensionless parameters k that characterizes the spectral function of the ohmic thermal baths, the operation of the quantum diode with both high rectification and significant heat current could be achieved by choosing a set of values $(\Delta,\omega_L,\omega_R,\delta T)$ that yields a high rectification factor and taking a high enough k. Therefore, despite of the tradeoff between the rectification factor and heat current, the optimal operation of the quantum diode can thus be achieved by favoring the optimization of R, through those four parameters.

For the sake of simplicity and clarity, in this work we have considered that both spins are aligned in the z direction, and thus it constitutes a first step towards more general cases, involving spins with arbitrary directions. In any case, the proposed quantum diode could be realized in practice using two interacting electrons or quantum dots embedded in a nanoparticle each [46,47]. These two nanoparticles can play the role of thermal baths, whose different temperatures could be controlled by electrical means. The desired coupling strength Δ could then be reached by modulating the distance between the nanoparticles deposited on a substrate.

IV. CONCLUSIONS

Based on the analytical solution of a master equation for the density matrix, we have shown that a quantum thermal diode can be built up with two interacting spinlike systems characterized by different excitation frequencies and coupled to a thermal bath each. Explicit expressions for both the heat current and rectification factor of the diode have been derived as well as the conditions for their optimization have been found. It has been shown that there exists a critical two-system's coupling proportional to the temperature of the hotter thermal bath, for which the magnitude of the heat current is maximum. The rectification ability of the diode increases with the ratio of excitation frequencies, which drives the asymmetry of the heat current.

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