Quantum counterpart of equipartition theorem in quadratic systems

Xin-Hai Tong [*]

Department of Physics, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa-shi, Chiba 277-8574, Japan

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The equipartition theorem is a fundamental law of classical statistical physics, which states that every degree of freedom contributes $k_\mathrm{B}T/2$ to the energy, where T is the temperature and k_B is the Boltzmann constant. Recent studies have revealed the existence of a quantum version of the equipartition theorem. In the present work, we focus on how to obtain the quantum counterpart of the generalized equipartition theorem for arbitrary quadratic systems in which the multimode Brownian oscillators interact with multiple reservoirs at the same temperature. An alternative method of deriving the energy of the system is also discussed and compared with the result of the quantum version of the equipartition theorem, after which we conclude that the latter is more reasonable. Our results can be viewed as an indispensable generalization of recent works on a quantum version of the equipartition theorem.

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I. INTRODUCTION

One of the elegant principles of classical statistical physics is the equipartition theorem, which has numerous applications in various topics, such as thermodynamics [1–3], astrophysics [4–6], and applied physics [7–9]. It is natural to consider the quantum version of the equipartition theorem, since quantum mechanics has been founded over a hundred years and so has quantum statistical mechanics.

Recent years have seen much progress on this topic. A novel work [10] investigated the simplest quantum Brownian oscillator model to formulate the energy of the system in terms of the average energy of a quantum oscillator in a harmonic well. Based on this work, more researchers [11–18] tried to study quantum counterparts of the equipartition theorem in different versions of quadratic open quantum systems from various perspectives, including electrical circuits [11], dissipative diamagnetism [18], and focusing on kinetic energy for a more general setup [19].

In this work, we aim to deduce a quantum counterpart of the generalized equipartition theorem [20] for arbitrary open quantum quadratic systems. Many quadratic systems share the same algebra $[\hat{A}, \hat{B}] = i\hbar$, where the binary operator pair can be the coordinate $\hat{x}$ and the momentum $\hat{p}$ for oscillators, the magnetic flux $\hat{\Phi}$ and the charge $\hat{Q}$ for quantum circuits, and so on. We here turn to Brownian oscillators as an example to grasp the physical nature of all these systems.

To construct such systems, we adopt a generalized Caldeira-Leggett model [21] and manage to transform it into a multimode Brownian-oscillator system that is well-discussed in Ref. [22]. For generality, we do not choose a concrete form of dissipation. We also generalize a formula in Ref. [23] for the internal energy so that it can be applied to the multimode Brownian oscillator system. It has been debated [24] which of the formulas in Ref. [23] or the quantum counterpart of the equipartition theorem given in Ref. [10] truly describes the energy of the system. Our analysis shows that the generalized version of the former formula cannot be used to find the energy, which implies that the latter one is more reasonable.

The remainder of this paper is organized as follows. In Sec. II, we construct a quadratic system from the Caldeira-Leggett model. In Sec. III we deduce the generalized equipartition theorem for this system and show its link to the conventional equipartition theorem. In Sec. IV we try to give a multimode version of the remarkable formula in Ref. [23]. More theoretical details are given in the Appendices. Numerical results are demonstrated in Sec. V. We summarize this paper in Sec. VI. Throughout this paper, we set $\hbar = 1$ and $\beta = 1/(k_\mathrm{B}T)$, with k_B being the Boltzmann constant and T being the temperature of the reservoirs if there is no special reminder.

II. ARBITRARY QUADRATIC SYSTEM

To construct our arbitrary quadratic system, let us start with the multimode Caldeira-Leggett model [21]:

$$H_\mathrm{CL} = \sum_u \frac{\hat{P}_u^2}{2M_u} + \sum_{uv} \frac{1}{2} k_{uv} \hat{Q}_u \hat{Q}_v + \sum_{\alpha j} \left[\frac{\hat{p}_{\alpha j}^2}{2m_{\alpha j}} + \frac{1}{2} m_{\alpha j} \omega_{\alpha j}^2 \left(\hat{x}_{\alpha j} + \frac{1}{m_{\alpha j}\omega_{\alpha j}^2} \sum_u c_{\alpha u j} \hat{Q}_u \right)^2 \right], \quad (1)$$

where $u, v \in \{1, 2, \ldots, n_\mathrm{S}\}$ and $j \in \{1, 2, \ldots, n_\alpha\}$ are indices for the oscillators in the system and in the αth bath, respectively. The coefficient $c_{\alpha u j}$ represents the coupling strength

[*] xinhai@iis.u-tokyo.ac.jp

between the coordinate of the uth oscillator in the system and the jth oscillator in the αth bath. The convention would put $-c_{\alpha uj}$ in the last term of Eq. (1), but we replace it by $c_{\alpha uj}$. We also have the commutation relations for all the momentum and position operators as follows:

$$[\hat{Q}_u, \hat{P}_v] = i\delta_{uv}, \quad [\hat{x}_{\alpha_1 j_1}, \hat{p}_{\alpha_2 j_2}] = i\delta_{\alpha_1\alpha_2}\delta_{j_1 j_2}, \tag{2}$$

with δ representing the Kronecker delta. Equation (1) can be reorganized in the following forms:

$$H_{\rm CL} = H_{\rm S} + H_{\rm SB} + h_{\rm B}, \tag{3a}$$

$$H_{\rm S} = \sum_u \frac{\hat{P}_u^2}{2M_u} + \frac{1}{2}\sum_{uv}\left(k_{uv} + \frac{c_{\alpha uj}c_{\alpha vj}}{m_{\alpha j}\omega_{\alpha j}^2}\right)\hat{Q}_u\hat{Q}_v, \tag{3b}$$

$$H_{\rm SB} = \sum_{\alpha u}\hat{Q}_u\hat{F}_{\alpha u}, \quad \hat{F}_{\alpha u} = \sum_j c_{\alpha uj}\hat{x}_{\alpha j}, \tag{3c}$$

$$h_{\rm B} = \sum_\alpha h_{\alpha\rm B} = \sum_{\alpha j}\left(\frac{\hat{p}_{\alpha j}^2}{2m_{\alpha j}} + \frac{1}{2}m_{\alpha j}\omega_{\alpha j}^2\hat{x}_{\alpha j}^2\right). \tag{3d}$$

Here, the system-bath interaction results from the linear coupling of the system coordinate $\hat{Q}_u$ and the random force $\hat{F}_{\alpha u}$. We also emphasize that all the mutually independent baths $\{h_{\alpha\rm B}\}$ in Eq. (3d) are at the same inverse temperature β. By defining the pure bath response function as

$$\boldsymbol{\phi}_\alpha(t) \equiv \left\{\phi_{\alpha uv}(t) \equiv i\langle[\hat{F}_{\alpha u}^{\rm B}(t), \hat{F}_{\alpha v}^{\rm B}(0)]\rangle_{\rm B}\right\}, \tag{4}$$

we recognize that

$$\sum_j \frac{c_{\alpha uj}c_{\alpha vj}}{m_{\alpha j}\omega_{\alpha j}^2} = \tilde{\phi}_{\alpha uv}(0), \tag{5}$$

where $\hat{F}_{\alpha u}^{\rm B}(t) \equiv e^{ih_{\rm B}t}\hat{F}_{\alpha u}e^{-ih_{\rm B}t}$ and the average is defined over the canonical ensembles of baths as in $\langle\cdots\rangle_{\rm B} := {\rm tr}_{\rm B}[\cdots\otimes_\alpha e^{-\beta h_{\alpha\rm B}}]/\prod_\alpha {\rm tr}_{\rm B}(e^{-\beta h_{\alpha\rm B}})$. In Eq. (5) we use a tilde to denote the Laplace transform $\tilde{f}(\omega) = \int_0^\infty {\rm d}\omega\, e^{i\omega t}f(t)$ for any function $f(t)$. By denoting $V_{uv} \equiv k_{uv} + \sum_\alpha \tilde{\phi}_{\alpha uv}(0)$ and $\Omega_u \equiv M_u^{-1}$ for convenience, we rewrite Eq. (3b) in the form

$$\begin{aligned} H_{\rm S} &= H_{\rm BO} + H_{\rm ren} \\ &\equiv \left[\frac{1}{2}\sum_u \Omega_u\hat{P}_u^2 + \frac{1}{2}\sum_{uv}\left(V_{uv} - \sum_\alpha\tilde{\phi}_{\alpha uv}(0)\right)\hat{Q}_u\hat{Q}_v\right] \\ &\quad + \left[\frac{1}{2}\sum_{\alpha uv}\tilde{\phi}_{\alpha uv}(0)\hat{Q}_u\hat{Q}_v\right], \end{aligned} \tag{6}$$

which is the starting point of our quantum counterpart of the equipartition theorem. Here, $H_{\rm ren}$ denotes the renormalization energy. The system Hamiltonian, referred to as Eq. (6), now is identical to the one presented in Ref. [22]. Physically, we need $\boldsymbol{V} = \{V_{uv}\}$, $\boldsymbol{k} = \{k_{uv}\}$, and $\boldsymbol{\Omega} = \{\Omega_u\delta_{uv}\}$ to be positive definite. Without loss of generality, we can always set $\boldsymbol{V}$ and $\boldsymbol{k}$ to be symmetric. The detailed derivation of Eq. (5) can be found in Appendix A.

III. QUANTUM COUNTERPART OF GENERALIZAD EQUIPARTITION THEOREM

The conventional quantum counterpart of the equipartition theorem for the single-mode Caldeira-Leggett model deals with the kinetic energy $E_{\rm k}(\beta)$ in the Gibbs state of the total system with the inverse temperature being β [10] in the form of

$$\begin{aligned} E_{\rm k}(\beta) &= \mathbb{E}_{\rm k}\left[\frac{\hbar\omega}{4}\coth\frac{\beta\hbar\omega}{2}\right] \\ &:= \int_0^\infty {\rm d}\omega\, \mathbb{P}_k(\omega)\frac{\hbar\omega}{4}\coth\frac{\beta\hbar\omega}{2}. \end{aligned} \tag{7}$$

Here, we temporarily add $\hbar$ for later convenience and $\mathbb{E}_{\rm k}[f(\omega)]$ denotes the expectation of a function $f(\omega)$ over the normalized distribution function $\mathbb{P}_{\rm k}(\omega)$, which satisifies $\mathbb{P}_{\rm k}(\omega) \geqslant 0$ and $\int_0^\infty {\rm d}\omega\, \mathbb{P}_{\rm k}(\omega) = 1$. Equation (7) can be reduced to the classical case since $\lim_{\hbar\to 0}E_{\rm k}(\beta) = \mathbb{E}_{\rm k}[\lim_{\hbar\to 0}(\hbar\omega/4)\coth(\hbar\beta\omega/2)] = \mathbb{E}_{\rm k}[1/2\beta] = 1/2\beta$. However, when some degrees of freedom are intertwined with each other, such as in our model [cf. Eq. (3)], it is better if we use the generalized equipartition theorem [20].

In the rest of this work, we study the quantity $\langle\hat{X}_i\partial H_{\rm BO}/\partial\hat{X}_j\rangle$ for any system degrees of freedom $\hat{X}_i, \hat{X}_j \in \{\hat{P}_u\}\cup\{\hat{Q}_u\}$, with the average defined in the total Gibbs state $\langle\cdots\rangle := {\rm tr}_{\rm T}[\ldots e^{-\beta H_{\rm CL}}]/{\rm tr}_{\rm T}\, e^{-\beta H_{\rm CL}}$, which is well-defined since we assume that all the baths are at the same inverse temperature β. The derivative of the operator here is merely a notation, indicating that we initially treat all distinct operators as mutually independent variables like real numbers. After obtaining the result, We restore these variables back to operators. In the main text we focus on the cases $\hat{X}_i = \hat{X}_j$, while other cases are discussed in Appendix C.

We have $\langle\hat{Q}_u\partial H_{\rm BO}/\partial\hat{Q}_u\rangle = \sum_v[V_{uv} - \sum_\alpha\tilde{\phi}_{\alpha uv}(0)]\langle\hat{Q}_u\hat{Q}_v\rangle$ when we choose $\hat{X}_i = \hat{X}_j = \hat{Q}_u$. With the help of the fluctuation-dissipation theorem [25] for the symmetrized correlation function [24], we obtain

$$\begin{aligned} &\frac{1}{2}\left\langle\left\{\hat{Q}_u, \frac{\partial H_{\rm BO}}{\partial\hat{Q}_u}\right\}\right\rangle \\ &\quad = \sum_v \frac{1}{\pi}\int_0^\infty {\rm d}\omega\left[V_{uv} - \sum_\alpha\tilde{\phi}_{\alpha uv}(0)\right]{\rm Re}\, J_{uv}^{QQ}(\omega)\coth\frac{\beta\omega}{2}, \end{aligned} \tag{8}$$

with $\boldsymbol{J}^{QQ}(\omega) = \{J_{uv}^{QQ}(\omega)\}$ being the anti-Hermitian part of the matrix $\tilde{\boldsymbol{\chi}}^{QQ}(\omega) = \{\tilde{\chi}_{uv}^{QQ}(\omega)\}$ and $\{\bullet, \circ\}$ representing the anti-commutator. Here, we denote the system response function of any two operators $\hat{A}_u$ and $\hat{B}_v$ as $\chi_{uv}^{AB}(t) \equiv i\langle[\hat{A}_u(t), \hat{B}_v(0)]\rangle$. According to Ref. [22], we also have some useful relations for the quantities like $\tilde{\boldsymbol{\chi}}^{AB}(\omega)$. We list them below for later convenience:

$$\tilde{\boldsymbol{\chi}}^{QQ}(\omega) = \left[\boldsymbol{\Omega}\boldsymbol{V} - \omega^2\mathbf{I} - \boldsymbol{\Omega}\sum_\alpha\tilde{\boldsymbol{\phi}}_\alpha(\omega)\right]^{-1}\boldsymbol{\Omega}, \tag{9a}$$

$$\tilde{\boldsymbol{\chi}}^{PP}(\omega) = \boldsymbol{\Omega}^{-1} + \omega^2\boldsymbol{\Omega}^{-1}\tilde{\boldsymbol{\chi}}^{QQ}(\omega)\boldsymbol{\Omega}^{-1}, \tag{9b}$$

$$\tilde{\boldsymbol{\chi}}^{QP}(\omega) = i\omega\tilde{\boldsymbol{\chi}}^{QQ}(\omega)\boldsymbol{\Omega}^{-1}, \tag{9c}$$

$$\tilde{\boldsymbol{\chi}}^{PQ}(\omega) = -i\omega\boldsymbol{\Omega}^{-1}\tilde{\boldsymbol{\chi}}^{QQ}(\omega), \tag{9d}$$

where $\boldsymbol{V}$ and $\boldsymbol{\Omega}$ are given below Eq. (6). Equation (8) can be recast as

$$\left\langle\hat{Q}_u\frac{\partial H_{\rm BO}}{\partial\hat{Q}_u}\right\rangle = \int_0^\infty {\rm d}\omega\, \mathbb{P}_{Q_uQ_u}(\omega)\frac{\omega}{2}\coth\frac{\beta\omega}{2}, \tag{10}$$

with

$$\mathbb{P}_{Q_uQ_u}(\omega) = \frac{2}{\pi\omega}\sum_v\left[V_{uv} - \sum_\alpha \tilde{\phi}_{\alpha uv}(0)\right]J^{QQ}_{uv}(\omega), \tag{11}$$

where we use the fact that $\boldsymbol{J}^{QQ}(\omega)$ is symmetric since $\tilde{\boldsymbol{\chi}}^{QQ}(\omega)$ is symmetric and therefore $\boldsymbol{J}^{QQ}(\omega)$ is real.

A similar process for the case $\hat{X}_i = \hat{X}_j = \hat{P}_u$ leads to $\langle\hat{P}_u\partial H_{\mathrm{BO}}/\partial\hat{P}_u\rangle = \Omega_u\langle\hat{P}_u^2\rangle$. Using the fluctuation-dissipation theorem [25] again, we find

$$\frac{1}{2}\left\langle\left\{\hat{P}_u, \frac{\partial H_{\mathrm{BO}}}{\partial\hat{P}_u}\right\}\right\rangle = \frac{\Omega_u}{\pi}\int_0^\infty \mathrm{d}\omega\ \mathrm{Re}\, J^{PP}_{uu}(\omega)\coth\frac{\beta\omega}{2}, \tag{12}$$

where $\boldsymbol{J}^{PP}(\omega) = \{J^{PP}_{uv}(\omega)\}$ is the anti-Hermitian part of matrix $\tilde{\boldsymbol{\chi}}^{PP}(\omega) = \{\tilde{\chi}^{PP}_{uv}(\omega)\}$ [cf. Eq. (9b)].

By substituting Eq. (9b) into Eq. (12), we obtain the final result

$$\left\langle\hat{P}_u\frac{\partial H_{\mathrm{BO}}}{\partial\hat{P}_u}\right\rangle = \int_0^\infty \mathrm{d}\omega\ \mathbb{P}_{P_uP_u}(\omega)\frac{\omega}{2}\coth\frac{\beta\omega}{2}, \tag{13}$$

with

$$\mathbb{P}_{P_uP_u}(\omega) = \frac{2\omega}{\pi\Omega_u}J^{QQ}_{uu}(\omega). \tag{14}$$

The proof of positivity and normalization of Eqs. (11) and (14) can be found in Appendix B, by which we can recast Eqs. (10) and (13) as

$$\left\langle\hat{X}_i\frac{\partial H_{\mathrm{BO}}}{\partial\hat{X}_i}\right\rangle = \mathbb{E}_{ii}\left[\frac{\omega}{2}\coth\frac{\beta\omega}{2}\right]$$
$$:= \int_0^\infty \mathrm{d}\omega\ \mathbb{P}_{X_iX_i}(\omega)\frac{\omega}{2}\coth\frac{\beta\omega}{2}, \tag{15}$$

with

$$\mathbb{P}_{ii}(\omega) \geqslant 0 \quad \text{and} \quad \int_0^\infty \mathrm{d}\omega\ \mathbb{P}_{ii}(\omega) = 1, \tag{16}$$

where we use the notation $\mathbb{P}_{ii}$ rather than $\mathbb{P}_{X_iX_i}$ for simplicity. In Appendix C, we extend Eqs. (15) and (16) to the cases where $\hat{X}_i \neq \hat{X}_j$ and we summarize all the results as

$$\frac{1}{2}\left\langle\left\{\hat{X}_i, \frac{\partial H_{\mathrm{BO}}}{\partial\hat{X}_j}\right\}\right\rangle = \mathbb{E}_{ij}\left[\frac{\hbar\omega}{2}\coth\frac{\hbar\beta\omega}{2}\right] \tag{17}$$

for any system degrees of freedom $\hat{X}_i, \hat{X}_j \in \{\hat{P}_u\} \cup \{\hat{Q}_u\}$ with

$$\mathbb{P}_{ii}(\omega) \geqslant 0 \quad \text{and} \quad \int_0^\infty \mathrm{d}\omega\ \mathbb{P}_{ij}(\omega) = \delta_{ij}, \tag{18}$$

and $\mathbb{E}_{ij}[\ldots]$ denotes the expectation over $\mathbb{P}_{ij}(\omega)$. Here, we temporarily add $\hbar$ for later convenience and let δ denote the Kronecker delta. Equations (17) and (18) are partly the main results of the present work.

Discussions are presented here to conclude this section. Once we take the classical limit $\hbar \to 0$ and the weak-coupling limit $c_{\alpha uj} \to 0$, Eq. (17) reduces to $\langle X_i\partial H_{\mathrm{S}}/\partial X_j\rangle = \delta_{ij}/\beta$ [cf. Eq. (6)], which is termed as the generalized equipartition theorem [20]. We also emphasize that though the right-hand side of Eq. (17) depends on different degrees of freedom (i and j), the function $(\omega/2)\coth(\beta\omega/2)$ is universal for all the degrees of freedom, which is the "equipartition" in a quantum sense. Therefore, Eq. (17) is termed as the quantum counterpart of the generalized equipartition theorem. It is evident that Eqs. (11) and (14) reduce to the results in Refs. [10,24] for the single-mode $n_{\mathrm{S}} = 1$ case. Besides, by noticing that $\langle\hat{P}_u\partial H_{\mathrm{BO}}/\partial\hat{P}_u\rangle$ equals twice the kinetic energy of the uth oscillator and $\boldsymbol{J}^{PP}(\omega) = \omega\boldsymbol{\Omega}^{-1}\boldsymbol{J}^{QQ}(\omega)\boldsymbol{\Omega}^{-1}$ [cf. Eq. (9b)], Eqs. (13) and (14) reduce to the results presented in Ref. [19].

Equation (17) here offers a new angle on how to calculate the quantities of open systems, which are generally hard to obtain. An application is given below. Noting that the total energy is given by $E(\beta) = 1/2\sum_i\langle\hat{X}_i\partial H_{\mathrm{BO}}/\partial\hat{X}_i\rangle$, we arrive at

$$E(\beta) = \mathbb{E}\left[\frac{n_{\mathrm{S}}\omega}{2}\coth\frac{\beta\omega}{2}\right], \tag{19}$$

with $\mathbb{E}[\ldots]$ denoting the expectation over

$$\mathbb{P}(\omega) := \sum_i \mathbb{P}_{ii}(\omega)/2n_{\mathrm{S}}, \tag{20}$$

which is checked [cf. Eq. (16)] to be nonnegative and normalized over $\mathbb{R}^+$. Equation (19) is termed as the quantum counterpart of conventional equipartition theorem [24]. Moving further with the help of thermodynamic equations, we can determine the free energy $F(\beta)$ of the system by

$$F(\beta) + \beta\frac{\partial F(\beta)}{\partial\beta} = E(\beta), \tag{21}$$

and hence Eqs. (21) and (19) may yield

$$F(\beta) = \mathbb{E}\left[\frac{n_{\mathrm{S}}}{\beta}\ln\left(2\sinh\frac{\beta\omega}{2}\right)\right], \tag{22}$$

from which we further obtain an expression for the partition function of the system in the form of

$$\ln Z_{\mathrm{S}}(\beta) = -\mathbb{E}\left[n_{\mathrm{S}}\ln\left(2\sinh\frac{\beta\omega}{2}\right)\right]. \tag{23}$$

Note that Eq. (23) is much easier to obtain than the conventional influence-functional approach [26,27].

IV. ALTERNATIVE APPROACH FOR THE ENERGY

A recent review [24] presented another approach to obtain the energy of the system of multimode harmonic oscillators. When introduced in Ref. [23], the result was only limited to the single-mode case. Here, we generalize their derivation and find that their derivation is not applicable to the multimode case.

The starting point of Ref. [23] is quite straightforward. Since the conventional definition for the internal energy of the oscillator $U_{\mathrm{S}}(\beta) = \mathrm{tr}_{\mathrm{T}}[H_{\mathrm{BO}}e^{-\beta H_{\mathrm{CL}}}]/\,\mathrm{tr}\,e^{-\beta H_{\mathrm{CL}}}$ is generally challenging to handle, we adopt normal-mode coordinates, so that the transformed Hamiltonian H_{T} describes $N(= 1 + \sum_\alpha n_\alpha)$ uncoupled oscillators. Physically we do not need to obtain the detailed information for any normal modes, since the total energy $U_{\mathrm{T}}(\beta)$ is only associated with the normal frequencies, namely,

$$U_{\mathrm{T}}(\beta) = \sum_{r=1}^N u(\overline{\omega}_r, \beta) := \sum_{r=1}^N \frac{\overline{\omega}_r}{2}\coth\frac{\beta\overline{\omega}_r}{2}, \tag{24}$$

with $\overline{\omega}_r$ being the normal frequency for the rth oscillator in the transformed system. Here, we also introduce the notation

$u(\omega, \beta) \equiv (\omega/2)\coth(\beta\omega/2)$ for later convenience. Since the energy for the independent bath is well-defined as

$$U_{\mathrm{B}}(\beta) = \sum_{\alpha j} \frac{\omega_{\alpha j}}{2} \coth \frac{\beta\omega_{\alpha j}}{2}, \tag{25}$$

the authors of Ref. [23] interpreted the difference

$$U_{\mathrm{S}}(\beta) = U_{\mathrm{T}}(\beta) - U_{\mathrm{B}}(\beta) \tag{26}$$

as the internal energy and found it to be

$$U_{\mathrm{S}}(\beta) = \int_0^\infty \mathrm{d}\omega \, \frac{1}{\pi} \, \mathrm{Im} \, \frac{\mathrm{d}}{\mathrm{d}\omega} \ln \tilde{\chi}^{QQ}(\omega) \frac{\omega}{2} \coth \frac{\beta\omega}{2}, \tag{27}$$

where $\tilde{\chi}^{QQ}(\omega)$ is the one-dimensional version of Eq. (9a).

Following their procedures for the multimode case, we find (see Appendix D for a detailed derivation)

$$U_{\mathrm{T}}(\beta) - n_{\mathrm{S}} U_{\mathrm{B}}(\beta) = \int_0^\infty \mathrm{d}\omega \, \mathbb{B}(\omega) n_{\mathrm{S}} \frac{\omega}{2} \coth \frac{\beta\omega}{2}, \tag{28}$$

with

$$\mathbb{B}(\omega) = \frac{1}{\pi n_{\mathrm{S}}} \, \mathrm{Im} \, \frac{\mathrm{d}}{\mathrm{d}\omega} \ln \det \tilde{\boldsymbol{\chi}}^{QQ}(\omega), \tag{29}$$

which does not give us $U_{\mathrm{S}}(\beta) = U_{\mathrm{T}}(\beta) - U_{\mathrm{B}}(\beta)$. On the other hand, the result of the system's internal energy according to the quantum counterpart of equipartition theorem [cf. Eq. (19)] is applicable to any multimode case. Therefore, we conclude that Eq. (19) is more reasonable than the alternative approach discussed in Ref. [23] as an expression for the internal energy of the system. Equations (28) and (29) are another part of the main results of this work.

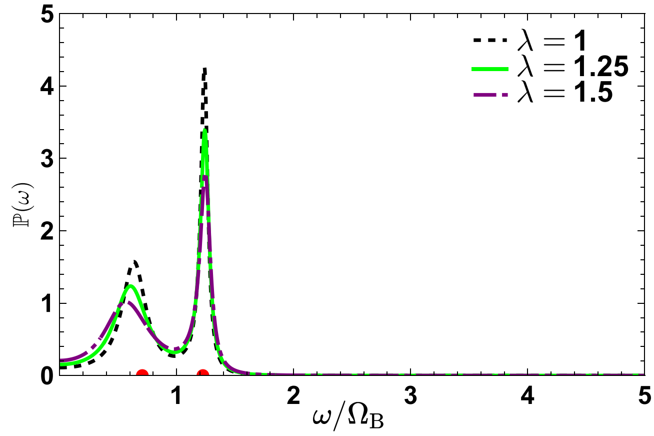
V. NUMERICAL DEMONSTRATIONS

In this section, we use the two-mode ($u, v \in \{1, 2\}$) Brownian-oscillator system coupled with one reservoir ($\alpha = 1$) to give a numerical demonstration of our results. The system Hamiltonian H_{S} of the two-mode system reads $H_{\mathrm{S}} = (\Omega_1 \hat{P}_1^2 + \Omega_2 \hat{P}_2^2)/2 + (V_{11}\hat{Q}_1^2 + V_{22}\hat{Q}_2^2 + 2V_{12}\hat{Q}_1\hat{Q}_2)/2$, while the system-bath interaction term becomes $H_{\mathrm{SB}} = \hat{Q}_1\hat{F}_1 + \hat{Q}_2\hat{F}_2$, with the random force $\hat{F}_{u1} = \sum_j c_{uj}\hat{x}_j$ for $u \in \{1, 2\}$. The bath Hamiltonian reduces to $h_{\mathrm{B}} = \sum_j (\hat{p}_j^2/2m_j + m_j\omega_j^2\hat{x}_j^2/2)$. To enhance clarity, we choose the spectrum of the pure bath in the following form:

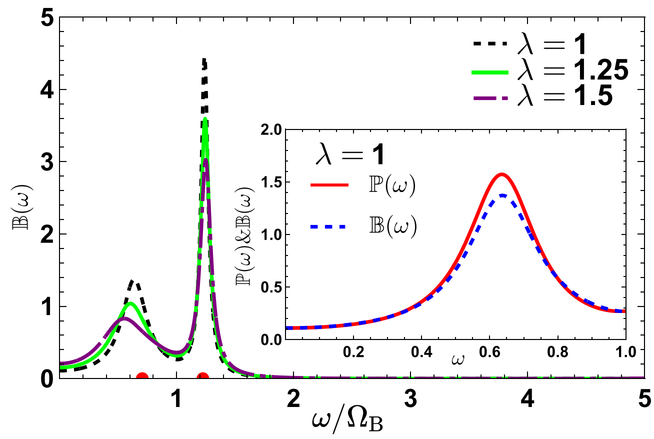
$$\tilde{\boldsymbol{\phi}}(\omega, \lambda) = \lambda \boldsymbol{\eta} \, \mathrm{Im} \, \frac{\Omega_{\mathrm{B}}^2}{\Omega_{\mathrm{B}}^2 - \omega^2 - i\omega\gamma_{\mathrm{B}}}, \tag{30}$$

with $\boldsymbol{\eta} \equiv \{\eta_{uv} = \eta_u \delta_{uv}\}$ specifying the strength of the system-bath couplings. From an experimental point of view, this setup can be realized, for example, in molecular junctions [28–30]. We also introduce the parameter $\lambda \in \{1, 1.25, 1.5\}$ to vary the strength, which can be realized experimentally by modifying the intermolecular distance. Through out this section, we select the parameters in the unit of Ω_{B} as $\gamma_{\mathrm{B}} = 1.25\,\Omega_{\mathrm{B}}$, $\Omega_1 = \Omega_2 = V_{11} = V_{22} = \Omega_{\mathrm{B}}$, and $V_{12} = V_{21} = 0.5\,\Omega_{\mathrm{B}}$. The strength of the couplings are chosen to be $\eta_1 = 0.2\,\Omega_{\mathrm{B}}$ and $\eta_2 = 0.1\,\Omega_{\mathrm{B}}$.

Figures 1(a) and 1(b) depict $\mathbb{P}(\omega)$ and $\mathbb{B}(\omega)$ in the three cases.



(a)



(b)

FIG. 1. Plots of $\mathbb{P}(\omega)$ in panel (a) and $\mathbb{B}(\omega)$ in panel (b) when $\lambda \in \{1, 1.25, 1.5\}$. Here the red dots on the horizontal axes represent $\omega = 0.7071\,\Omega_{\mathrm{B}}$ and $\omega = 1.224\,\Omega_{\mathrm{B}}$, respectively, which are the square root of eigenvalues of the matrix $\boldsymbol{\Omega V}$ according to the parameters chosen in the main text.

As λ decreases, the curves become sharper around the square root of the eigenvalues of $\boldsymbol{\Omega V}$. In other words, the maximum points of $\mathbb{P}(\omega)$ and $\mathbb{B}(\omega)$ become closer to them as λ decreases. In fact, we can prove the following (see Appendix E):

$$\lim_{\{c_{\alpha uj}\} \to \{0\}} \mathbb{P}(\omega) = \frac{1}{n_{\mathrm{S}}} \sum_{\omega_i^2 \in \mathrm{spec}(\boldsymbol{\Omega V})} [\delta(\omega - \omega_i) + \delta(\omega + \omega_i)], \tag{31}$$

where the summation is over all the square roots of eigenvalues of the matrix $\boldsymbol{\Omega V}$ (considering multiplicity). These results show that, in the weak-coupling limit, only the oscillators with these typical frequencies contribute to the quantity that we consider, such as the energy. In this case, the energy reads

$$E_{\mathrm{weak}}(\beta) = \sum_{\omega_i^2 \in \mathrm{spec}(\boldsymbol{\Omega V})} \frac{\omega_i}{2} \coth \frac{\beta\omega_i}{2}, \tag{32}$$

which is how the quantum counterpart of the equipartition theorem behaves in the weak-coupling limit. In the single-mode case, a similar pattern has also been discussed in Ref. [24].

VI. SUMMARY

To summarize, we derived a quantum counterpart of the generalized equipartition for arbitrary quadratic systems, which we can also reduce to the results presented in previous works for the single-mode case. We also extended another formula for the internal energy of the multimode Brownian-oscillator system. The generalized formula and our analysis shed light on the controversies of the method. We noticed that our quantum counterpart of the equipartition theorem can be used to obtain the partition function of the system in a much easier way than the classical approach [27]. Our results can be viewed as an indispensable development of recent works on the quantum counterpart of the equipartition theorem.

As a future prospect, expressing thermodynamic quantities as an infinite series also offers potential advantages for this objective [24]. Work in this direction is in progress. Furthermore, it seems difficult to discuss the quantum version of the equipartition theorem without the help of the fluctuation-dissipation theorem and to consider it over steady states or even in general nonequilibrium. Discussing the present topic under other more difficult setups, such as quartic systems, is also challenging. All of them constitute directions of further development.

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APPENDIX A: DERIVATION OF Eq. (5)

Here we show the detailed derivation of Eq. (5). Let us start from the Heisenberg equation of motion for any operator, $\dot{\hat{X}}(t) = i[H_{\mathrm{T}}, \hat{X}(t)]$. Focusing on the bath quantities $\hat{x}_{\alpha j}$ and $\hat{p}_{\alpha j}$, we obtain

$$\dot{\hat{x}}_{\alpha j}(t) = \hat{p}_{\alpha j}(t)/m_{\alpha j}, \tag{A1a}$$

$$\dot{\hat{p}}_{\alpha j}(t) = -m_{\alpha j}\omega_{\alpha j}^2 \hat{x}_{\alpha j}(t) - \sum_u c_{\alpha u j}\hat{Q}_u(t). \tag{A1b}$$

Taking the time derivative of Eq. (A1a) and putting Eq. (A1b) into it, we obtain the following equation:

$$\ddot{\hat{x}}_{\alpha j}(t) = -\omega_{\alpha j}^2 \hat{x}_{\alpha j}(t) - \sum_u \frac{c_{\alpha u j}}{m_{\alpha j}}\hat{Q}_u(t). \tag{A2}$$

One can verify the formal solution to Eq. (A2) is

$$\hat{x}_{\alpha j}(t) = \hat{x}_{\alpha j}(0)\cos\omega_{\alpha j}t + \frac{\hat{p}_{\alpha j}(0)}{m_{\alpha j}\omega_{\alpha j}}\sin\omega_{\alpha j}t + \sum_u \frac{c_{\alpha u j}}{m_{\alpha j}\omega_{\alpha j}}\int_0^t \mathrm{d}\tau\, \sin\omega_{\alpha j}(t-\tau)\hat{Q}_u(\tau). \tag{A3}$$

Meanwhile, we know from the definition of $\hat{F}^{\mathrm{B}}_{\alpha u}$ that

$$\hat{F}^{\mathrm{B}}_{\alpha u}(t) = \sum_j c_{\alpha u j}\left[\hat{x}_{\alpha j}(0)\cos\omega_{\alpha j}t + \frac{\hat{p}_{\alpha j}(0)}{m_{\alpha j}\omega_{\alpha j}}\sin\omega_{\alpha j}t\right]. \tag{A4}$$

Putting Eq. (A4) into Eq. (4), we directly obtain

$$\phi_{\alpha uv}(t) = \sum_j \frac{c_{\alpha u j}c_{\alpha v j}}{m_{\alpha j}\omega_{\alpha j}}\sin\omega_{\alpha j}t$$
$$\Rightarrow \tilde{\phi}_{\alpha uv}(\omega) = \sum_j \frac{c_{\alpha u j}c_{\alpha v j}}{m_{\alpha j}\omega_{\alpha j}}\frac{\omega_{\alpha j}}{-\omega^2+\omega_{\alpha j}^2}. \tag{A5}$$

Thus, obviously we find Eq. (5). We can also see that $\tilde{\boldsymbol{\phi}}_\alpha(\omega)$ is a symmetric matrix.

APPENDIX B: PROOF OF POSITIVITY AND NORMALIZATION

From the positivity of $\boldsymbol{J}^{QQ}(\omega)$ [31], we directly know $\mathbb{P}_{P_uP_u}(\omega) \geqslant 0$. Once we rewrite Eq. (11) as $\mathbb{P}_{Q_uQ_u}(\omega) = 2\{[\boldsymbol{V} - \sum_\alpha \tilde{\boldsymbol{\phi}}_\alpha(0)]\boldsymbol{J}^{QQ}(\omega)\}_{uu}/\pi\omega$ (note that $\boldsymbol{J}^{QQ}(\omega)$ is symmetric), its positivity becomes evident, since $\boldsymbol{k} \equiv \boldsymbol{V} - \sum_\alpha \tilde{\boldsymbol{\phi}}_\alpha(0)$ and $\boldsymbol{J}^{QQ}(\omega)$ is also positive definite [31]. For the normalization of $\mathbb{P}_{Q_uQ_v}(\omega)$, we notice the following relation (cf. Eq. (2.17) in Ref. [31]):

$$\tilde{\chi}^{QQ}_{uv}(0) = \frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\frac{J^{QQ}_{uv}(\omega)}{\omega}. \tag{B1}$$

One can notice that $J^{QQ}_{uv}(\omega)$ is an odd function, since $J^{QQ}_{uv}(-\omega) = -J^{QQ}_{vu}(\omega)$ [31] and $\boldsymbol{J}^{QQ}(\omega)$ is symmetric. We further obtain from Eq. (B1) that

$$\left\{\left[\boldsymbol{V} - \sum_\alpha \tilde{\boldsymbol{\phi}}_\alpha(0)\right]^{-1}\right\}_{uv} = \tilde{\chi}^{QQ}_{uv}(0) = \frac{2}{\pi}\int_0^{\infty}\mathrm{d}s\,\frac{J^{QQ}_{uv}(\omega)}{\omega}, \tag{B2}$$

where the first equality comes from Eq. (9a). Equation (B2) is equivalent to

$$\delta_{uw} = \sum_v \frac{2}{\pi}\int_0^\infty \mathrm{d}\omega\,\frac{J^{QQ}_{uv}(\omega)}{\omega}\left[\boldsymbol{V} - \sum_\alpha \tilde{\boldsymbol{\phi}}_\alpha(0)\right]_{vw}. \tag{B3}$$

In the special case of $u = w$ and considering the symmetry of $\boldsymbol{V}$, $\tilde{\boldsymbol{\phi}}_\alpha(0)$, and $\tilde{\boldsymbol{\chi}}^{QQ}(\omega)$, we can deduce that $\int_0^\infty \mathrm{d}\omega\,\mathbb{P}_{Q_uQ_u}(\omega) = 1$.

As for $\mathbb{P}_{P_uP_u}(\omega)$, from Eq. (2.17) in Ref. [31] we obtain

$$\dot{\chi}^{QQ}_{uv}(0) = \frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\omega J^{QQ}_{uv}(\omega). \tag{B4}$$

We can also know from Ref. [22] that $\dot{\boldsymbol{\chi}}^{QQ}(t) = -\boldsymbol{\Omega}\boldsymbol{\chi}^{QP}(t)$. Letting $t = 0$, we obtain $\dot{\boldsymbol{\chi}}^{QQ}(0) = \boldsymbol{\Omega}$ since $\chi^{QP}_{uv}(0) = i\langle[\hat{Q}_u, \hat{P}_v]\rangle = \delta_{uv}$. Using this result and Eq. (B4), we arrive at

$\int_{-\infty}^{\infty} \mathrm{d}\omega\, \omega J_{uv}^{QQ}(\omega) = \pi\Omega_u\delta_{uv}$. By observing that $J_{uv}^{QQ}(\omega)$ is an odd function, we can further deduce the following:

$$2\int_0^{\infty} \mathrm{d}\omega\, \omega J_{uv}^{QQ}(\omega) = \pi\Omega_u\delta_{uv}, \tag{B5}$$

which in the case of $u = v$ is equivalent to $\int_0^{\infty}\mathrm{d}\omega\, \mathbb{P}_{P_uP_u}(\omega)=1$, and thus we finish the proof for the normalization of $\mathbb{P}_{P_uP_u}(\omega)$.

APPENDIX C: ANALYSIS OF THE CASES $\hat{X}_i \neq \hat{X}_j$

In this section we complete the derivation of our quantum counterpart of the generalized equipartition theorem by considering the cases of $\hat{X}_i \neq \hat{X}_j$. We start from

$$\begin{aligned}\frac{1}{2}\left\langle\left\{\hat{P}_u, \frac{\partial H_{\mathrm{BO}}}{\partial \hat{P}_v}\right\}\right\rangle &= \frac{1}{2}\Omega_v\langle\{\hat{P}_u, \hat{P}_v\}\rangle\\ &= \frac{1}{2}\Omega_v\frac{2}{\pi}\int_0^{\infty}\mathrm{d}\omega\, \mathrm{Re}J_{uv}^{PP}(\omega)\coth\frac{\beta\omega}{2}\\ &= \frac{1}{\pi\Omega_u}\int_0^{\infty}\mathrm{d}\omega\, \omega^2 J_{uv}^{QQ}(\omega)\coth\frac{\beta\omega}{2}\\ &= \int_0^{\infty}\mathrm{d}\omega\, \mathbb{P}_{P_uP_v}(\omega)\frac{\omega}{2}\coth\frac{\beta\omega}{2},\end{aligned} \tag{C1}$$

with

$$\mathbb{P}_{P_uP_v}(\omega) = \frac{2\omega}{\pi\Omega_u}J_{uv}^{QQ}(\omega), \tag{C2}$$

where in the third line we use the fact that $\boldsymbol{J}^{PP}(\omega) = \{J_{uv}^{PP}(\omega)\}$ and $\boldsymbol{J}^{QQ}(\omega) = \{J_{uv}^{QQ}(\omega)\}$ are the anti-Hermitian parts of Eqs. (9b) and (9a), respectively. Using Eq. (B5) we obtain

$$\int_0^{\infty}\mathrm{d}\omega\, \mathbb{P}_{P_uP_v}(\omega) = \delta_{uv}. \tag{C3}$$

Similarly, we evaluate

$$\begin{aligned}&\frac{1}{2}\left\langle\left\{\hat{Q}_u, \frac{\partial H_{\mathrm{BO}}}{\partial \hat{Q}_v}\right\}\right\rangle\\ &= \frac{1}{2}\sum_w\left[V_{vw} - \sum_\alpha\tilde{\phi}_{\alpha vw}(\omega)\right]\langle\{\hat{Q}_u, \hat{Q}_w\}\rangle\\ &= \frac{1}{2}\sum_w\frac{2}{\pi}\int_0^{\infty}\mathrm{d}\omega\left[V_{vw} - \sum_\alpha\tilde{\phi}_{\alpha vw}(\omega)\right]\\ &\quad\times \mathrm{Re}\, J_{uw}^{QQ}(\omega)\coth\frac{\beta\omega}{2}\\ &= \int_0^{\infty}\mathrm{d}\omega\, \mathbb{P}_{Q_uQ_v}(\omega)\frac{\omega}{2}\coth\frac{\beta\omega}{2},\end{aligned} \tag{C4}$$

with

$$\mathbb{P}_{Q_uQ_v}(\omega) = \frac{2}{\pi\omega}\sum_w\left[V_{vw} - \sum_\alpha\tilde{\phi}_{\alpha vw}(\omega)\right]J_{uw}^{QQ}(\omega). \tag{C5}$$

By utilizing Eq. (B3), we can derive the following result:

$$\int_0^{\infty}\mathrm{d}\omega\, \mathbb{P}_{Q_uQ_v}(\omega) = \delta_{uv}. \tag{C6}$$

As an additional outcome, we can also express Eqs. (C2) and (C6) in the following alternative forms: $\mathbb{P}_{P_uP_v}(\omega) = 2\omega[\boldsymbol{J}^{QQ}(\omega)\dot{\boldsymbol{\chi}}^{-1}(0)]_{uv}/\pi$ and $\mathbb{P}_{Q_uQ_v}(\omega) = 2[\boldsymbol{J}^{QQ}(\omega)\boldsymbol{\chi}^{-1}(0)]_{uv}/\omega\pi$, respectively.

Then we consider

$$\begin{aligned}\frac{1}{2}\left\langle\left\{\hat{Q}_u, \frac{\partial H_{\mathrm{BO}}}{\partial \hat{P}_v}\right\}\right\rangle &= \frac{1}{2}\Omega_v\langle\{\hat{Q}_u, \hat{P}_v\}\rangle\\ &= \frac{\Omega_v}{\pi}\int_0^{\infty}\mathrm{d}\omega\, \mathrm{Re}\, J_{uv}^{QP}(\omega)\coth\frac{\beta\omega}{2}\\ &= \int_0^{\infty}\mathrm{d}\omega\, \mathbb{P}_{Q_uP_v}(\omega)\frac{\omega}{2}\coth\frac{\beta\omega}{2},\end{aligned} \tag{C7}$$

with

$$\mathbb{P}_{Q_uP_v}(\omega) = \frac{2\Omega_v}{\pi\omega}\mathrm{Re}\, J_{uv}^{QP}(\omega), \tag{C8}$$

where $\boldsymbol{J}^{QP}(\omega) = \{J_{uv}^{QP}(\omega)\}$ is the anti-Hermitian part of the matrix $\tilde{\boldsymbol{\chi}}^{QP}(\omega) = \{\tilde{\chi}_{uv}^{QP}(\omega) = \int_0^{\infty}\mathrm{d}\omega\, e^{i\omega t}\chi_{uv}^{QP}(t)\}$. By Eq. (9c), we derive $\boldsymbol{J}^{QP}(\omega) = \omega[\tilde{\boldsymbol{\chi}}^{QQ}(\omega)\boldsymbol{\Omega}^{-1} + \boldsymbol{\Omega}^{-1}\tilde{\boldsymbol{\chi}}^{QQ\dagger}(\omega)]/2$, which helps us to deduce

$$\int_0^{\infty}\mathrm{d}\omega\, \mathbb{P}_{Q_uP_v}(\omega) = 0. \tag{C9}$$

Here, we utilized the property that $\tilde{\boldsymbol{\chi}}^{QQ}(\omega)$ is an even function in order to establish the following useful equality: $\int_0^{\infty}\mathrm{d}\omega\, \tilde{\boldsymbol{\chi}}^{QQ}(\omega) = \int_{-\infty}^{\infty}\mathrm{d}\omega\, \tilde{\boldsymbol{\chi}}^{QQ}(\omega)/2 = \boldsymbol{\chi}^{QQ}(0) = \mathbf{0}$, which together with the expression for $\boldsymbol{J}^{QP}(\omega)$ helps us to obtain Eq. (C9). Following a similar process, we deduce

$$\begin{aligned}&\frac{1}{2}\left\langle\left\{\hat{P}_u, \frac{\partial H_{\mathrm{BO}}}{\partial \hat{Q}_v}\right\}\right\rangle\\ &= \frac{1}{2}\sum_w\left[V_{vw} - \sum_\alpha\tilde{\phi}_{\alpha vw}(\omega)\right]\langle\{\hat{P}_u, \hat{Q}_w\}\rangle\\ &= \sum_w\frac{1}{\pi}\left[V_{vw} - \sum_\alpha\tilde{\phi}_{\alpha vw}(\omega)\right]\\ &\quad\times\int_0^{\infty}\mathrm{d}\omega\, \mathrm{Re}\, J_{uw}^{QP}(\omega)\coth\frac{\beta\omega}{2}\\ &= \int_0^{\infty}\mathrm{d}\omega\, \mathbb{P}_{P_uQ_v}(\omega)\frac{\omega}{2}\coth\frac{\beta\omega}{2},\end{aligned} \tag{C10}$$

with

$$\mathbb{P}_{uv}^{PQ}(\omega) = \frac{2}{\pi\omega}\sum_w\left[V_{vw} - \sum_\alpha\tilde{\phi}_{\alpha vw}(\omega)\right]\mathrm{Re}\, J_{uw}^{PQ}(\omega), \tag{C11}$$

where $\boldsymbol{J}^{PQ}(\omega) = \{J_{uv}^{PQ}(\omega)\}$ is the anti-Hermitian part of the matrix $\tilde{\boldsymbol{\chi}}^{PQ}(\omega) = \{\tilde{\chi}_{uv}^{PQ}(\omega) = \int_0^{\infty}\mathrm{d}\omega\, e^{i\omega t}\chi_{uv}^{PQ}(t)\}$. From Eq. (9d) we obtain $\boldsymbol{J}^{PQ}(\omega) = -\omega[\boldsymbol{\Omega}^{-1}\tilde{\boldsymbol{\chi}}^{QQ}(\omega) + \tilde{\boldsymbol{\chi}}^{QQ\dagger}(\omega)\boldsymbol{\Omega}^{-1}]/2$, which also gives us

$$\int_0^{\infty}\mathrm{d}\omega\, \mathbb{P}_{P_uQ_v}(\omega) = 0, \tag{C12}$$

since $\int_0^{\infty}\mathrm{d}\omega\, \tilde{\boldsymbol{\chi}}^{QQ}(\omega) = \mathbf{0}$. Summarizing Eqs. (C1), (C3), (C4), (C6), (C7), (C9), (C10), and (C12) and the results of the cases of $\hat{X}_i = \hat{X}_j$ in the main text, we finally obtain Eqs. (17) and (18).

APPENDIX D: ALTERNATIVE APPROACH FOR THE ENERGY

To obtain Eqs. (28) and (29) for the multimode case, we set $N = n_{\rm S} + \sum_\alpha n_\alpha$ and follow the procedures in Ref. [23].

(i) From a normal-mode analysis we obtain the following relation between $\tilde{\boldsymbol{\chi}}^{QQ}(\omega)$ and all the normal frequencies $\{\varpi_r\}$:

$$\det \tilde{\boldsymbol{\chi}}^{QQ}(\omega) = (-1)^{n_{\rm S}} \det \boldsymbol{\Omega} \frac{\prod_{\alpha j}\left(\omega^2 - \omega_{\alpha j}^2\right)}{\prod_{r=1}^{N}\left(\omega^2 - \varpi_r^2\right)}, \tag{D1}$$

whose derivation is presented hereafter.

Applying a similar treatment as in Appendix A to $\hat{Q}_u(t)$ and $\hat{P}_u(t)$, we obtain

$$\ddot{\hat{Q}}_u(t) + \sum_v \Omega_v V_{uv} \hat{Q}_u(t) + \sum_{\alpha j} \Omega_u c_{\alpha u j} \hat{x}_{\alpha j}(t) = 0. \tag{D2}$$

Let

$$\hat{Q}_u(t) = \overline{Q}_u(\varpi) e^{-i\varpi t}, \quad \hat{x}_{\alpha j}(t) = \overline{x}_{\alpha j}(\varpi) e^{-i\varpi t}, \tag{D3}$$

where ϖ is the normal frequency. To perform a normal-mode analysis, we put Eq. (D3) into Eqs. (A2) and (D2), finding

$$-\varpi^2 \overline{Q}_u(\varpi) + \sum_v \Omega_v V_{uv} \overline{Q}_v(\varpi) + \sum_{\alpha j} \Omega_u c_{\alpha u j} \overline{x}_{\alpha j}(\varpi) = 0, \tag{D4a}$$

$$-\varpi^2 \overline{x}_{\alpha j}(\varpi) + \omega_{\alpha j}^2 \overline{x}_{\alpha j}(\varpi) + \sum_v \frac{c_{\alpha u j}}{m_{\alpha j}} \overline{Q}_u(\varpi) = 0. \tag{D4b}$$

Solving Eq. (D4b) for $\overline{x}_{\alpha j}(\varpi)$ and substituting it into Eq. (D4a), we obtain

$$\sum_v \left[-\varpi^2 \delta_{uv} + \Omega_v \delta_{uv} + \sum_{\alpha j} \Omega_u \frac{c_{\alpha u j} c_{\alpha v j}}{m_{\alpha j}\left(\varpi^2 - \omega_{\alpha j}^2\right)} \right] \overline{Q}_v(\varpi) = 0. \tag{D5}$$

To obtain nontrivial normal frequencies, we require [cf. Eq. (A5)]

$$\det\left[\boldsymbol{\Omega V} - \varpi^2 \mathbf{I} - \boldsymbol{\Omega} \sum_\alpha \tilde{\boldsymbol{\phi}}_\alpha(\varpi) \right] = 0, \tag{D6}$$

which is also an equation for all the normal frequencies $\{\varpi\}$. As a function with respect to ω^2 [cf. Eqs. (9a) and (A5)], $\det \tilde{\boldsymbol{\chi}}^{QQ}(\omega)$ has singular points at all $\{\omega_r^2\}$ and zero points at all $\{\omega_{\alpha j}^2\}$. Therefore, we can write $\det \tilde{\boldsymbol{\chi}}^{QQ}(\omega)$ in the form of Eq. (D1). Note that $n_{\rm S}$ is the dimension of the matrix and the factor $(-1)^{n_{\rm S}}$ comes from the change of sign in the determinant.

(ii) Once we denote $\mathcal{A}(z) \equiv \det \tilde{\boldsymbol{\chi}}^{QQ}(z^{1/2})$, mathematically it is easy to know

$$\frac{\mathrm{d}}{\mathrm{d}z}[\mathcal{A}(z)]^{-1}\bigg|_{z=\varpi_r^2} = \operatorname{Res}\left[\mathcal{A}(z), \varpi_r^2\right]^{-1}, \tag{D7}$$

which helps us to recast Eq. (24) as

$$U_{\rm T}(\beta) = \sum_{r=1}^{N} u(\varpi_r, \beta) \frac{\mathrm{d}}{\mathrm{d}z}[\mathcal{A}(z)]^{-1}\bigg|_{z=\varpi_r^2} \operatorname{Res}\left[\mathcal{A}(z), \varpi_r^2\right]. \tag{D8}$$

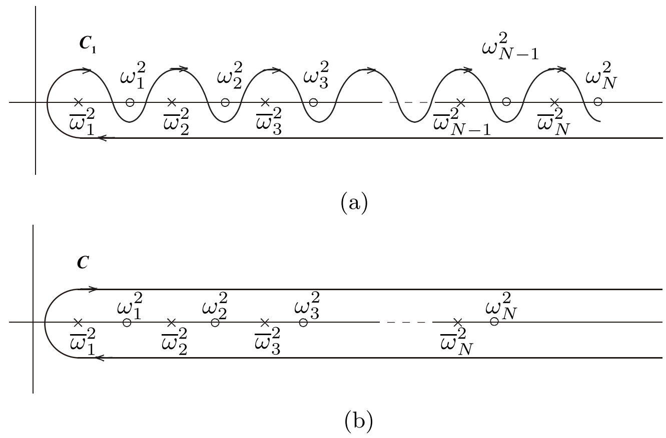

FIG. 2. Plots of (a) the contour C_1 and (b) the contour C. Here $\{\omega_1^2, \omega_2^2, \ldots\}$ denote elements in $\{\omega_{\alpha j}^2\}$.

By the residue theorem we further write Eq. (D8) as

$$U_{\rm T}(\beta) = -\frac{1}{2\pi i} \int_{C_1} \mathrm{d}z\, u(z^{1/2}, \beta) \frac{\mathrm{d}}{\mathrm{d}z}[\mathcal{A}(z)]^{-1} \mathcal{A}(z), \tag{D9}$$

where the contour C_1 is shown in Fig. 2(a).

(iii) In order to change the contour C_1 into C [see Fig. 2(b)], we need to consider a set of clockwise circle contours $C_{\alpha j} : |z - \omega_{\alpha j}^2| = \epsilon$. Since $C = C_1 + \sum_{\alpha j} C_{\alpha j}$ and we have

$$\begin{aligned} &\sum_{\alpha j} \int_{|z-\omega_{\alpha j}^2|=\epsilon} \mathrm{d}z\, u(z^{1/2}, \beta) \frac{\mathrm{d}}{\mathrm{d}z}[\mathcal{A}(z)]^{-1} \mathcal{A}(z) \\ &\quad = 2\pi i n_{\rm S} \sum_{\alpha j} \frac{\omega_{\alpha j}}{2} \coth \frac{\beta \omega_{\alpha j}}{2}, \end{aligned} \tag{D10}$$

the derivation of Eq. (D10) is straightforward as long as we remember [cf. Eq. (9a)]

$$\begin{aligned} \mathcal{A}(z) &\equiv \det \tilde{\boldsymbol{\chi}}^{QQ}(z^{1/2}) \\ &= \det \boldsymbol{\Omega} / \det\left[\boldsymbol{\Omega V} - z\mathbf{I} - \boldsymbol{\Omega} \sum_\alpha \tilde{\boldsymbol{\phi}}_\alpha(z^{1/2}) \right] \\ &:= (-1)^{n_{\rm S}} \det \boldsymbol{\Omega} / \det \boldsymbol{C}(z), \end{aligned} \tag{D11}$$

where we define

$$\boldsymbol{C}(z) \equiv z\mathbf{I} - \boldsymbol{\Omega V} - \boldsymbol{\Omega} \sum_{\alpha j} \boldsymbol{c}_{\alpha j} \frac{\omega_{\alpha j}}{z - \omega_{\alpha j}^2} \tag{D12}$$

for simplification. Thus,

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}z}[\mathcal{A}(z)]^{-1} \mathcal{A}(z) \\ &\quad = (-1)^{n_{\rm S}} (\det \boldsymbol{\Omega})^{-1} \frac{\mathrm{d}}{\mathrm{d}z} \det \boldsymbol{C}(z) \times (-1)^{n_{\rm S}} \det \boldsymbol{\Omega} / \det \boldsymbol{C}(z) \\ &\quad = \det \boldsymbol{C}(z) \operatorname{tr}\left[\boldsymbol{C}^{-1}(z) \frac{\mathrm{d}}{\mathrm{d}z} \boldsymbol{C}(z) \right] / \det \boldsymbol{C}(z) \\ &\quad = \operatorname{tr}\left[\boldsymbol{C}^{-1}(z) \frac{\mathrm{d}}{\mathrm{d}z} \boldsymbol{C}(z) \right]. \end{aligned} \tag{D13}$$

By noting that

$$\frac{\mathrm{d}}{\mathrm{d}z}\det \boldsymbol{C}(z) = \det \boldsymbol{C}(z)\,\mathrm{tr}\left[\boldsymbol{C}^{-1}(z)\frac{\mathrm{d}}{\mathrm{d}z}\boldsymbol{C}(z)\right], \tag{D14}$$

we find

$$\begin{aligned}
\boldsymbol{C}^{-1}(z)\frac{\mathrm{d}}{\mathrm{d}z}\boldsymbol{C}(z) &= \left[z\mathbf{I} - \boldsymbol{\Omega V} - \boldsymbol{\Omega}\sum_{\alpha j}\boldsymbol{c}_{\alpha j}\frac{\omega_{\alpha j}}{z-\omega_{\alpha j}^2}\right]^{-1}\left[\mathbf{I} + \boldsymbol{\Omega}\sum_{\alpha j}\boldsymbol{c}_{\alpha j}\frac{\omega_{\alpha j}}{(z-\omega_{\alpha j}^2)^2}\right]\\
&= \left[z\mathbf{I} - \boldsymbol{\Omega V} - \boldsymbol{\Omega}\sum_{\alpha j}\boldsymbol{c}_{\alpha j}\frac{\omega_{\alpha j}}{z-\omega_{\alpha j}^2}\right]^{-1}\frac{1}{(z-\omega_{\beta k}^2)^2}\\
&\quad\times\left[(z-\omega_{\beta k}^2)^2\mathbf{I} + \boldsymbol{\Omega}\boldsymbol{c}_{\beta k}\omega_{\beta k} + \boldsymbol{\Omega}\sum_{\alpha j\neq\beta k}\boldsymbol{c}_{\alpha j}\omega_{\alpha j}\frac{(z-\omega_{\beta k}^2)^2}{(z-\omega_{\alpha j}^2)^2}\right]\\
&= \left[z(z-\omega_{\beta k}^2)^2\mathbf{I} - \boldsymbol{\Omega V}(z-\omega_{\beta k}^2)^2 - \boldsymbol{\Omega}\boldsymbol{c}_{\beta k}\omega_{\beta k}(z-\omega_{\beta k}^2) - \boldsymbol{\Omega}\sum_{\alpha j\neq\beta k}\boldsymbol{c}_{\alpha j}\omega_{\alpha j}\frac{(z-\omega_{\beta k}^2)^2}{z-\omega_{\alpha j}^2}\right]^{-1}\\
&\quad\times\left[(z-\omega_{\beta k}^2)^2\mathbf{I} + \boldsymbol{\Omega}\boldsymbol{c}_{\beta k}\omega_{\beta k} + \boldsymbol{\Omega}\sum_{\alpha j\neq\beta k}\boldsymbol{c}_{\alpha j}\omega_{\alpha j}\frac{(z-\omega_{\beta k}^2)^2}{(z-\omega_{\alpha j}^2)^2}\right]\\
&\overset{\lim_{z\to\omega_{\beta k}^2}}{=} \left[-\boldsymbol{\Omega}\boldsymbol{c}_{\beta k}\omega_{\beta k}(z-\omega_{\beta k}^2)\right]^{-1}(\boldsymbol{\Omega}\boldsymbol{c}_{\beta k}\omega_{\beta k})\\
&= -\frac{1}{z-\omega_{\beta k}^2}\mathbf{I}.
\end{aligned} \tag{D15}$$

Evaluating Eq. (D10) using Eqs. (D13) and (D15) gives us Eq. (D10). By Eq. (25) we deduce the following expression:

$$U_\mathrm{T}(\beta) - n_\mathrm{S}U_\mathrm{B}(\beta) = -\frac{1}{2\pi i}\int_C \mathrm{d}z\, u(z^{1/2},\beta)\frac{\mathrm{d}}{\mathrm{d}z}[\mathcal{A}(z)]^{-1}\mathcal{A}(z). \tag{D16}$$

(iv) First we set $z=\omega^2$ in Eq. (D16). Then by noticing that $\tilde{\boldsymbol{\chi}}^{QQ}(\omega) = [\tilde{\boldsymbol{\chi}}^{QQ}(-\omega)]^*$ [31] and the function $u(\omega,\beta)$ is even with respect to ω, we simplify Eq. (D16) to obtain the final remarkable expression:

$$U_\mathrm{T}(\beta) - n_\mathrm{S}U_\mathrm{B}(\beta) = \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega\, u(\omega,\beta)\,\mathrm{Im}\,\frac{\mathrm{d}}{\mathrm{d}\omega}\ln\det \boldsymbol{\chi}^{QQ}(\omega). \tag{D17}$$

Equation (D17) can also be recast to the form of the equipartition theorem:

$$U_\mathrm{T}(\beta) - n_\mathrm{S}U_\mathrm{B}(\beta) = \int_0^\infty \mathrm{d}\omega\, \mathbb{B}(\omega)\frac{\omega}{2}\coth\frac{\beta\omega}{2}, \tag{D18}$$

where

$$\mathbb{B}(\omega) = \frac{1}{\pi n_\mathrm{S}}\,\mathrm{Im}\,\frac{\mathrm{d}}{\mathrm{d}\omega}\ln\det\tilde{\boldsymbol{\chi}}^{QQ}(\omega). \tag{D19}$$

Therefore we obtain Eqs. (28) and (29), which reduce to Eq. (26) when $n_\mathrm{S}=1$.

APPENDIX E: PROOF OF Eq. (31) IN THE MAIN TEXT

In this section we give a proof of Eq. (31). From Eqs. (11), (14), and (20) we obtain

$$\begin{aligned}
\mathbb{P}(\omega) &= \frac{1}{2n_\mathrm{S}}\sum_u[\mathbb{P}_{Q_uQ_u}(\omega) + \mathbb{P}_{P_uP_u}(\omega)]\\
&= \frac{1}{2n_\mathrm{S}}\sum_u\left\{\frac{2}{\pi\omega}\sum_v\left[V_{uv} - \sum_\alpha\tilde{\phi}_{\alpha uv}(0)\right]J_{uv}^{QQ}(\omega)\right.\\
&\qquad\left.+\frac{2\omega}{\pi\Omega_u}J_{uu}^{QQ}(\omega)\right\}\\
&= \frac{1}{\pi n_\mathrm{S}\omega}\,\mathrm{tr}\left\{\left[\boldsymbol{V} - \sum_\alpha\tilde{\boldsymbol{\phi}}_\alpha(0) + \omega^2\boldsymbol{\Omega}^{-1}\right]\boldsymbol{J}^{QQ}(\omega)\right\}\\
&= \frac{1}{\pi n_\mathrm{S}\omega}\,\mathrm{tr}\left\{\left[\boldsymbol{V} - \sum_\alpha\tilde{\boldsymbol{\phi}}_\alpha(0) + \omega^2\boldsymbol{\Omega}^{-1}\right]\right.\\
&\qquad\left.\times\,\mathrm{Im}\left[\boldsymbol{\Omega V} - \omega^2\mathbf{I} - \boldsymbol{\Omega}\sum_\alpha\tilde{\boldsymbol{\phi}}_\alpha(\omega)\right]^{-1}\right\}.
\end{aligned} \tag{E1}$$

In the weak-coupling limit, all $c_{\alpha uj}\to 0$, and therefore $\boldsymbol{\phi}_\alpha(\omega)\to\mathbf{0}$ [cf. Eq. (A5)]. Equation (E1) becomes

$$\begin{aligned}
\mathbb{P}(\omega) &= \frac{1}{\pi n_\mathrm{S}\omega}\,\mathrm{tr}[(\boldsymbol{V} + \omega^2\boldsymbol{\Omega}^{-1})\,\mathrm{Im}(\boldsymbol{\Omega V} - \omega^2\mathbf{I})^{-1}]\\
&= \begin{cases} 0, & \text{if } \boldsymbol{\Omega V} - \omega^2\mathbf{I} \text{ is invertible,}\\ \infty, & \text{if } \boldsymbol{\Omega V} - \omega^2\mathbf{I} \text{ is not invertible,}\end{cases}
\end{aligned} \tag{E2}$$

but we still know from the normalization of $\mathbb{P}_{Q_uQ_u}(\omega)$ and $\mathbb{P}_{P_uP_u}(\omega)$ that

$$\int_0^\infty d\omega\, \mathbb{P}(\omega) = 1. \tag{E3}$$

Equation (E2) is always 0 except for the square root of the eigenvalues of the matrix $\boldsymbol{\Omega V}$. Considering Eq. (E3) and the definition for the Dirac delta function, we obtain

$$\lim_{\{c_{\alpha uj}\}\to\{0\}} \mathbb{P}(\omega) = \frac{1}{n_\mathrm{S}} \sum_{\omega_i^2\in\mathrm{spec}(\boldsymbol{\Omega V})} \delta(\omega-\omega_i), \quad \omega>0, \tag{E4}$$

where the summation is over all the square roots of eigenvalues of the matrix $\boldsymbol{\Omega V}$ (considering multiplicity). The coefficients $1/n_\mathrm{S}$ come from the numbers of the positive eigenvalues of $\boldsymbol{\Omega V}$, which equals n_S due to the fact that $\boldsymbol{\Omega V}$ and $\sqrt{\boldsymbol{\Omega}}\boldsymbol{V}\sqrt{\boldsymbol{\Omega}}$ are similar and the latter is a positive definite matrix of dimension n_S. Since $\boldsymbol{J}^{QQ}(\omega)$ is odd [31], it follows that $\mathbb{P}(\omega)$ is an even function, as indicated by the penultimate equality in Eq. (E1). With this we obtain Eq. (31).

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