Exact time-averaged thermal conductance for small systems: Comparison between direct calculation and Green-Kubo formalism

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In this paper, we study exactly the thermal conductance for a low dimensional system represented by two coupled massive Brownian particles, both directly and via a Green-Kubo expression. Both approaches give exactly the same result. We also obtain exactly the steady-state probability distribution for that system by means of time averaging.

I. INTRODUCTION

Exact results, in physics, play an important and useful role as a reference for other methods. For instance, they can be used to study specific features of models which are not easily accessible to approximative methods, such as computer simulations. However, nontrivial exact results are few and difficult to come by: in the literature of transport phenomena there are not many exact calculations for transport coefficients based on the mechanical parameters of the systems under observation [1–9]. Indeed, the calculation of transport coefficients is one of the most important goals of nonequilibrium physics.

In fact, the rigorous derivation of Fourier's law for bulk Hamiltonian systems is still under debate [2]. The soluble harmonic models used to evaluate the thermal conductance do not reproduce the necessary scattering of the energy unless local thermal reservoirs (which act in part as effective scatterers for the energy incoming on them) are coupled to the bulk sites. Other models such as mass disordered ones have been proposed but there is evidence that mass disorder alone will not give rise to Fourier's law in two dimensions [1]. The presence of anharmonicity on the coupling level would probably be sufficient for energy to scatter and diffuse from site to neighboring site. However, the technical details for obtaining exact rigorous results are, as far as we know, too difficult to overcome at the present level [2].

On the other hand, for equilibrium statistical mechanics the probability distribution for a given system can be found, given that it obeys Liouville's theorem [10] and the external macroscopic constraints [11], by means of an ensemble of points in phase space when that system is ergodic. However, ergodicity is not a necessary condition for obtaining the long times of the stationary probability distribution since it is always possible, at least in principle, to obtain the time average for any physical quantity during the realization of an actual experiment.

What distinguishes time averaging from other exact methods derived from the solution of a Fokker-Planck formalism is that time averaging can take into account, exactly, all the orders of the moments of the dynamical variables. The Fokker-Planck formalism is exact only to the second-order moments while time average is akin to the stationary solution of the Kramers-Moyal equation that is correct at all orders of moments [12]. For simplicity's sake we use Gaussian white noise in the present work but the method is readily generalizable to any type of noise given that all its moments are known.

Our present goal is to study exactly the validity and consistency of some methods used in the derivation of transport coefficients (namely, the thermal conductance) for small classical systems. The reasons for using small systems in our model are many fold. First, exact calculations become feasible. Second, macroscopic transport properties associated with large systems must have a mechanical counterpart in small systems. Macroscopic flows of mass, momentum, or energy are the effects of the averaging of the action of microscopic forces and work. Third, small systems are interesting per se. There are difficulties inherent to small systems due to the fact that one cannot take the thermodynamic limit that averages out many problems associated with solving the dynamics of large systems, similarly to the law of large numbers that arises from the summation of many random variables [13]. We can also take into account exactly the effects of the inertia and of a possible non-Markovian nature for the noise.

For deriving the exact time-averaged thermal conductance, we choose a simple system which is capable of nontrivially transmitting heat between its constitutive parts, via mechanical work, when subjected to a gradient of (white-noise) temperature: a system of two coupled Brownian particles (BP) with the coupling constant k acting as the sole information channel between the particles. In the present case, the system dynamics is linear and the linear-response treatment shall be proven to be exact, as we will see in the following.

We can apply a method previously used by the authors [14,15] to the study of thermal conduction between the

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coupled BP system. The exact time-averaging method of Refs. [14,15] is capable of obtaining exactly the stationary probability distribution for Brownian particles submitted to white and colored noises. In particular, by submitting a single massive BP to two different thermal contacts, at distinct temperatures (similarly to some glasses that are subjected to thermal vibrations and structural modifications represented by distinct noise functions at different time scales [16]), we can keep it from reaching thermal equilibrium [15].

Since the present model is effectively zero dimensional, the thermal conductance between the Brownian particles is defined simply as the energy flow per unit time per temperature difference between the particles, i.e., the conductive flow of energy (for particle 1, from particle 2) is defined as $j_{1,2} = -\kappa(T_{1,2} - T_{2,1})$, where κ is the interparticle thermal conductance in first-order approximation. Indeed, there have been some recent developments in treating finite systems that can be adapted to the problem under study [17,18]. In that case, the transport coefficient κ is obtained via a convenient Green-Kubo (GK) formulation. The calculation of the transport coefficients by this method can be an interesting starting point for the study of more complex models, such as polymers subjected to gradients of temperature [2,5,9]. It will also provide an important test for the choice of flow variable appropriate for such models. However, in order to avoid the rather artificial construction of an ensemble of reservoirs that need to be coupled to the particles along the linear polymer (harmonic crystal), a generalization of the method will be needed to include nonlinearities on the potential. This way, a much more realistic picture of thermal conduction will be obtained.

The thermal conductance between two particles is not a well defined macroscopic quantity since we are far from the thermodynamic limit and cannot define a macroscopic (and diffusive) flow of heat. However, it is clear that if a (classic) macroscopic system is partitioned into two parts, energy conduction is realized by the interactions (work) at the interface.

Furthermore, we add a periodic variation in the temperature of the Brownian particles. This is an interesting effect that can lead to the appearance of currents for systems presenting asymmetries in the potential energy [19,20]. Periodic oscillations of different types are capable of creating currents [21,22] in the case of zero average forces acting on the particles. The combination of ratchet-type potential energy and periodic time oscillation for the temperature has been extensively studied [20,23].

This paper is organized as follows: in Sec. II we define the model. In Sec. III we explain the method of time averaging and show the main contributions to the probability distribution. In Sec. IV we calculate the time-averaged steady-state distribution for the nonequilibrium conditions. In Sec. V we obtain the thermal conductance and in Sec. VI we discuss our main conclusions.

II. EXACTLY SOLVABLE MODEL

Our model consists of two massive BP coupled by a harmonic potential and subjected to white noise at distinct temperatures. This could be interpreted as two atoms in a crystal, coupled by a harmonic potential.

Despite the reduced number of variables, the present system contains the main ingredients of more complex models. In it, we can define the energy transfer as the microscopical work, which in macroscopical systems becomes the internally transferred heat. In the following, we describe the model in detail and, using time-average techniques [14,15], we calculate exactly the probability distribution for the relevant Brownian variables.

A. Langevin-type equation

The system composed of two coupled punctual and massive BPs is described by the equations:

$$\dot{x}_\alpha(t) = v_\alpha(t), \tag{1}$$

$$m_\alpha \dot{v}_\alpha(t) = -k[x_\alpha(t) - x_\beta(t)] - k' x_\alpha(t) - \gamma_\alpha v_\alpha(t) + \eta_\alpha(t). \tag{2}$$

Gaussian behavior is to be expected for the probability distribution for the time-averaged stationary state, according to previous published works (see especially Secs. 1.3.E.2 and 2.2.E.2 in Ref. [24]).

For simplicity, we make: $m_1 = m_2 = m$, $k'' = k'$, and $\gamma_1 = \gamma_2 = \gamma$. Thus the equations can be written as

$$m\ddot{x}_\alpha(t) = -k[x_\alpha(t) - x_\beta(t)] - k' x_\alpha(t) - \gamma \dot{x}_\alpha(t) + \eta_\alpha(t), \tag{3}$$

where $\alpha, \beta = 1, 2$, $\alpha \neq \beta$, and the initial conditions are

$$x_1(0) = x_2(0) = v_1(0) = v_2(0) = 0.$$

B. Noise properties

Both white Gaussian noise terms can be defined in terms of their two lowest two cumulants:

$$\langle \eta_\alpha(t) \rangle = 0, \tag{4}$$

$$\langle \eta_\alpha(t) \eta_\beta(t') \rangle = 2\gamma T_\alpha(t) \delta_{\alpha\beta} \delta(t - t'), \tag{5}$$

where the modulated temperatures above are given by

$$T_\alpha(t) = \bar{T}_\alpha [1 + A_\alpha \sin(\omega_\alpha t)]^2, \tag{6}$$

for $\alpha = 1, 2$ and $|A_\alpha| < 1$.

The oscillating temperatures, in other models, can induce very interesting effects such as sending heat fluxes against gradients of temperature [23] or directed fluxes of particles in periodic potentials [19,20,25–27].

C. Laplace transformations

Taking the Laplace transformations of Eqs. (1) and (2) yields

$$(ms^2 + \gamma s + k + k') \tilde{x}_1(s) = k \tilde{x}_2(s) + \tilde{\eta}_1(s), \tag{7}$$

$$\tilde{v}_1(s) = s \tilde{x}_1(s), \tag{8}$$

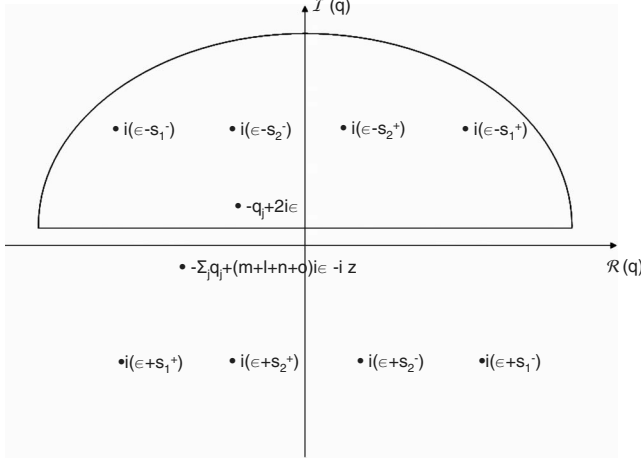$$(ms^2 + \gamma s + k + k') \tilde{x}_2(s) = k \tilde{x}_1(s) + \tilde{\eta}_2(s), \tag{9}$$

FIG. 1. Integration path for the equilibrium distribution, Eq. (19).

$$\tilde{v}_2(s) = s\tilde{x}_2(s). \tag{10}$$

Defining $\Gamma(s) \equiv ms^2 + \gamma s + k + k'$ and rearranging Eqs. (7)–(10), one finds that

$$\tilde{x}_1(s) = \Lambda(s)\tilde{\eta}_1(s) + \Delta(s)\tilde{\eta}_2(s), \tag{11}$$

$$\tilde{v}_1(s) = s\Lambda(s)\tilde{\eta}_1(s) + s\Delta(s)\tilde{\eta}_2(s), \tag{12}$$

$$\tilde{x}_2(s) = \Delta(s)\tilde{\eta}_1(s) + \Lambda(s)\tilde{\eta}_2(s), \tag{13}$$

$$\tilde{v}_2(s) = s\Delta(s)\tilde{\eta}_1(s) + s\Lambda(s)\tilde{\eta}_2(s), \tag{14}$$

where

$$\Lambda(s) \equiv \frac{\Gamma(s)}{\Gamma^2(s) - k^2}, \tag{15}$$

$$\Delta(s) \equiv \frac{k}{\Gamma^2(s) - k^2}. \tag{16}$$

The Laplace transformation for the independent noise variables is given by ($\alpha = 1, 2$):

$$
\frac{\langle \tilde{\eta}_\alpha(iq_i + \epsilon)\tilde{\eta}_\alpha(iq_j + \epsilon)\rangle}{2\gamma\bar{T}_\alpha}
$$
$$
= \left[\frac{1}{i(q_i + q_j) + 2\epsilon} + \frac{2A_\alpha\omega_\alpha}{[i(q_i + q_j) + 2\epsilon]^2 + \omega_\alpha^2}\right.
$$
$$
\left. + \frac{2A_\alpha^2\omega_\alpha^2}{[i(q_i + q_j) + 2\epsilon]\{[i(q_i + q_j) + 2\epsilon]^2 + 4\omega_\alpha^2\}}\right]. \tag{17}
$$

All integration paths are the same and shown in Fig. 1.

III. PROBABILITY DISTRIBUTION

Here we show some of the steps (more details can be found in Refs. [14,15]) to obtain the expression for the instantaneous probability distribution for the system of coupled Brownian particles.

Time averaging, for a supposedly convergent distribution, is defined and calculated as in Refs. [14,15]:

$$\bar{f} = \lim_{\Omega \to \infty} \frac{1}{\Omega}\int_0^\Omega dt f(t) = \lim_{z \to 0^+} z\int_0^\infty dt e^{-zt} f(t).$$

From the definition for the instantaneous probability distribution:

$$
p(x_1, v_1, x_2, v_2, t)
$$
$$
= \langle \delta[x_1 - x_1(t)]\delta[v_1 - v_1(t)]\delta[x_2 - x_2(t)]\delta[v_2 - v_2(t)]\rangle, \tag{18}
$$

it is possible to show that [14,15] (more details to be found at [28]):

$$
p^{ss}(x_1, v_1, x_2, v_2) = \lim_{z \to 0} \lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} \frac{dQ_1}{2\pi}\frac{dQ_2}{2\pi}\frac{dP_1}{2\pi}\frac{dP_2}{2\pi} e^{iQ_1 x_1 + iP_1 v_1 + iQ_2 x_2 + iP_2 v_2}
$$
$$
\times \sum_{l,m,n,o=0}^{\infty} \frac{(-iQ_1)^l}{l!}\frac{(-iP_1)^m}{m!}\frac{(-iQ_2)^n}{n!}\frac{(-iP_2)^o}{o!} \int_{-\infty}^{+\infty} \prod_{f=1}^{l}\frac{dq_{1f}}{2\pi}\prod_{h=1}^{m}\frac{dp_{1h}}{2\pi} \int_{-\infty}^{+\infty} \prod_{j=1}^{n}\frac{dq_{2j}}{2\pi}\prod_{k=1}^{o}\frac{dp_{2k}}{2\pi}
$$
$$
\times \frac{z^{m+o+1}}{z - \left[\sum_{a=1}^{l}(iq_{1a} + \epsilon) + \sum_{b=1}^{m}(ip_{1b} + \epsilon) + \sum_{c=1}^{n}(iq_{2c} + \epsilon) + \sum_{d=1}^{o}(ip_{2d} + \epsilon)\right]}
$$
$$
\times \left\langle \prod_{f=1}^{l}\tilde{x}_1(iq_{1f} + \epsilon)\prod_{h=1}^{m}\tilde{v}_1(ip_{1h} + \epsilon)\prod_{j=1}^{n}\tilde{x}_2(iq_{2j} + \epsilon)\prod_{k=1}^{o}\tilde{v}_2(iq_{2k} + \epsilon)\right\rangle, \tag{19}
$$

where the integration paths for the (q, p) variables are given in Fig. 1.

An interesting case is the study of the average $\langle x_1^2(t) \rangle$. The time periodicity of the noise $[T_{1,2}(t+\mathcal{T})=T_{1,2}(t)]$ gets translated into a periodicity of distribution $[p(x,t+\mathcal{T})=p(x,t)]$, and by consequence also of the averages for the variables, e.g., $\langle x_1^2(t+\mathcal{T}) \rangle = \langle x_1^2(t) \rangle$. This is consistent with a Fokker-Planck treatment of the distribution found in the literature [19,20,25–27]. We now show that the instantaneous distribution described by Eq. (19) is indeed consistent with periodicity in time.

From Ref. [20], it is clear that $\langle x_1^2(t) \rangle$ is periodic in time with period $\mathcal{T}$:

$$\langle x_1^2(t+\mathcal{T}) \rangle = \int dx_1 p(x_1, t+\mathcal{T}) x_1^2 = \int dx_1 p(x_1,t) x_1^2 = \langle x_1^2(t) \rangle,$$

where the periodicity of the probability distribution directly implies that of the average. We assume that $T_2=0, k=0$ so the present model and the one from [20] coincide.

The average (for long time, after the memory of the initial conditions has already faded out) reads

$$\langle x_1^2(t) \rangle = \int dx_1 p(x_1,t) x_1^2$$

$$= \lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} \frac{dq_1}{2\pi} \frac{dq_2}{2\pi} e^{t[iq_1+iq_2+2\epsilon]} \langle \tilde{x}_1(iq_1+\epsilon) \tilde{x}_1(iq_2+\epsilon) \rangle.$$

By integrating the last equation above over the poles of $\langle \tilde{\eta}_1 \tilde{\eta}_2 \rangle$, we observe that, apart from the term of order $O(A^0)$, the terms carrying the contribution from the sine bring a dependence such that $iq_1+iq_2+2\epsilon = \pm i\omega$. By obtaining the residue, we are left with exponential terms of the form $e^{\pm i\omega t}$, which are periodic in time with period $\mathcal{T}$.

An interesting aspect of periodically varying noise is that it modulates the time behavior of distributions and averages, i.e., there are no stationary constant values for any of the moments of the Brownian variables: the moments are periodic functions of time. In this case, the time average we use corresponds to averages of these quantities taken over a period of the noise for very long observation times. In general lines, the next steps consist of expressing the Laplace transforms for the dynamical variables (x,v) into functions of the averages of the Laplace transforms of the noise.

IV. TIME-AVERAGED STEADY STATE DISTRIBUTION

A. Contributing terms

The main contributions for the probability shown in Eq. (19) coming from a typical integration are of the form [14,15,28]:

$$C_{\tilde{\alpha}_r \tilde{\beta}_s} = \int_0^\infty \frac{dq_i}{2\pi} \frac{dq_j}{2\pi} \frac{z}{z-i(q_i+q_j+2\epsilon+\oslash)}$$

$$\times \langle \tilde{\alpha}_r(iq_i+\epsilon) \tilde{\beta}_s(iq_j+\epsilon) \rangle, \quad (20)$$

where $\oslash = [\Sigma_{a=1, a \neq i}^l (iq_a+\epsilon) + \Sigma_{b=1, b \neq j}^n (iq_b+\epsilon)]$, $\alpha, \beta = x, v$, and $r, s = 1, 2$.

To understand what causes a term in Eq. (19) to contribute to the time-averaged steady-state probability distribution, it is necessary to observe that for a typical integration, such as the above term, there is a factor $I(z)$,

$$I(z) = \frac{z}{z-i(q_i+q_j+2\epsilon+\oslash)},$$

which, in the limit $z \to 0$, will vanish if there is a presence of any finite terms on its denominator (due to the residue calculations around the poles of the rest of the integrand). Only integrations that eliminate all the pairs of q's in the denominator of $I(z)$ will transform it into $I(z)=z/z=1$. This is a necessary condition for any of the integrations done below to contribute to the probability distribution. Each integration brings the corresponding multiplicative factors that need to be dealt with.

We define

$$Q_{\Lambda\Lambda} = \frac{k+k'}{4\gamma(k'^2+2kk')} + \frac{\gamma}{4[mk^2+(k+k')\gamma^2]}, \quad (21)$$

$$Q_{\Delta\Delta} = \frac{k^2[m(k+k')+\gamma^2]}{4\gamma k'(2k+k')[mk^2+(k+k')\gamma^2]}, \quad (22)$$

$$Q_{\Delta\Lambda} = Q_{\Lambda\Delta} = \frac{k}{4\gamma k'(2k+k')}, \quad (23)$$

$$\mathcal{R}_{\Lambda\Lambda} = \frac{1}{4} \left\{ \frac{mk^2+2(k+k')\gamma^2}{mk^2+(k+k')\gamma^2} \right\}, \quad (24)$$

$$\mathcal{R}_{\Delta\Delta} = \frac{1}{4} \left\{ \frac{mk^2}{mk^2+(k+k')\gamma^2} \right\}, \quad (25)$$

$$\mathcal{H} = \frac{k\gamma}{4[mk^2+\gamma^2(k+k')]}. \quad (26)$$

Thus, the contributing terms will be [28]:

$$C_{\tilde{x}_1 \tilde{x}_1} = \frac{z}{z-i\oslash} \{ \gamma \bar{T}_1 (2+A_1^2) Q_{\Lambda\Lambda} + \gamma \bar{T}_2 (2+A_2^2) Q_{\Delta\Delta}, \}, \quad (27)$$

$$C_{\tilde{x}_2 \tilde{x}_2} = \frac{z}{z-i\oslash} \{ \gamma \bar{T}_1 (2+A_1^2) Q_{\Delta\Delta} + \gamma \bar{T}_2 (2+A_2^2) Q_{\Lambda\Lambda}, \}, \quad (28)$$

$$C_{\tilde{x}_1 \tilde{x}_2} = \frac{z}{z-i\oslash} \{ \gamma \bar{T}_1 (2+A_1^2) + \gamma \bar{T}_2 (2+A_2^2) \} Q_{\Delta\Lambda}, \quad (29)$$

$$C_{\tilde{v}_1 \tilde{v}_1} = \frac{z}{z-i\oslash} \left\{ \frac{\bar{T}_1}{m}(2+A_1^2) \mathcal{R}_{\Lambda\Lambda} + \frac{\bar{T}_2}{m}(2+A_2^2) \mathcal{R}_{\Delta\Delta} \right\}, \quad (30)$$

$$C_{\tilde{v}_2 \tilde{v}_2} = \frac{z}{z-i\oslash} \left\{ \frac{\bar{T}_1}{m}(2+A_1^2) \mathcal{R}_{\Delta\Delta} + \frac{\bar{T}_2}{m}(2+A_2^2) \mathcal{R}_{\Lambda\Lambda} \right\}, \quad (31)$$

$$C_{\tilde{x}_1\tilde{v}_2} = \frac{z}{z-i\oslash}\mathcal{H}[\bar{T}_1(2+A_1^2) - \bar{T}_2(2+A_2^2)], \qquad (32)$$

$$C_{\tilde{x}_2\tilde{v}_1} = \frac{z}{z-i\oslash}\mathcal{H}[\bar{T}_2(2+A_2^2) - \bar{T}_1(2+A_1^2)]. \qquad (33)$$

The other possible terms vanish:

$$C_{\tilde{v}_1\tilde{v}_2} = C_{\tilde{x}_1\tilde{v}_1} = C_{\tilde{x}_2\tilde{v}_2} = 0, \qquad (34)$$

since they are integrations of products of odd functions of q's with even functions of q's.

Notice that the effect of modulation is to scale the temperature value by a factor of $1+A^2/2$. This is exactly what is obtained by taking the time average of $T[1+A\sin(\omega t)]^2$:

$$\overline{T[1+A\sin(\omega t)]^2} = T(1+A^2/2). $$

We notice that the coupling term k is responsible for the nonzero values of $\mathcal{Q}_{\Lambda\Delta}$, $\mathcal{Q}_{\Delta\Delta}$, $\mathcal{R}_{\Delta\Delta}$, and $\mathcal{H}$.

B. Exact solution for the time-averaged steady-state distribution

Using the results obtained above, it is possible to obtain that Eq. (19) is

$$p^{ss}(x_1,v_1,x_2,v_2) = \int_{-\infty}^{+\infty} \frac{dQ_1}{2\pi}\frac{dQ_2}{2\pi}\frac{dP_1}{2\pi}\frac{dP_2}{2\pi}$$
$$\times e^{iQ_1x_1+iP_1v_1+iQ_2x_2+iP_2v_2}\mathcal{W}(Q_1,P_1,Q_2,P_2),$$
$$(35)$$

where [28]

$$\mathcal{W}(Q_1,P_1,Q_2,P_2) = \sum_{M=0}^{\infty}\sum_{N=0}^{\infty}\sum_{S=0}^{\infty}\sum_{T=0}^{\infty}\frac{(iQ_1)^M}{M!}\frac{(iQ_2)^N}{N!}\frac{(iP_1)^S}{S!}\frac{(iP_2)^T}{T!}\langle\tilde{x}_1^M\tilde{x}_2^N\tilde{v}_1^S\tilde{v}_2^T\rangle$$

$$= \exp\{-\mathcal{H}[\bar{T}_1(2+A_1^2) - \bar{T}_2(2+A_2^2)][Q_1P_2 - Q_2P_1]\}\exp\left\{-\left(\frac{Q_1^2\mathcal{Q}_{\Lambda\Lambda} + 2Q_1Q_2\mathcal{Q}_{\Delta\Lambda} + Q_2^2\mathcal{Q}_{\Delta\Delta}}{2}\right)[\gamma\bar{T}_1(2+A_1^2)]\right.$$

$$\left. -\left(\frac{Q_2^2\mathcal{Q}_{\Lambda\Lambda} + 2Q_1Q_2\mathcal{Q}_{\Delta\Lambda} + Q_1^2\mathcal{Q}_{\Delta\Delta}}{2}\right)[\gamma\bar{T}_2(2+A_2^2)]\right\}\exp\left\{-\frac{P_1^2}{2}\left[\frac{\bar{T}_1}{m}(2+A_1^2)\mathcal{R}_{\Lambda\Lambda} + \frac{\bar{T}_2}{m}(2+A_2^2)\mathcal{R}_{\Delta\Delta}\right]\right\}$$

$$\times\exp\left\{-\frac{P_2^2}{2}\left[\frac{\bar{T}_1}{m}(2+A_1^2)\mathcal{R}_{\Delta\Delta} + \frac{\bar{T}_2}{m}(2+A_2^2)\mathcal{R}_{\Lambda\Lambda}\right]\right\}.$$
$$(36)$$

The exact final result is given by

$$p^{ss}(x_1,v_1,x_2,v_2) = \mathcal{G}_0\exp\{\mathcal{N}_{x_1x_1}x_1^2 + \mathcal{N}_{x_2x_2}x_2^2 + \mathcal{N}_{v_1v_1}v_1^2$$
$$+ \mathcal{N}_{v_2v_2}v_2^2 + \mathcal{N}_{x_1v_1}x_1v_1 + \mathcal{N}_{x_1x_2}x_1x_2$$
$$+ \mathcal{N}_{x_1v_2}x_1v_2 + \mathcal{N}_{x_2v_1}x_2v_1 + \mathcal{N}_{x_2v_2}x_2v_2$$
$$+ \mathcal{N}_{v_1v_2}v_1v_2\}, \qquad (37)$$

where all the coefficients $\mathcal{N}_{\alpha_r\beta_s}$ above depend on the temperatures and mechanical constants of the system.

Due to the couplings present in Eq. (37), it does not describe a usual Boltzmann distribution but instead a steady state where couplings between position and moments arise. The basic reason for this to occur is that the work done by the coupling spring is of the form (work done on particle 1 by the spring) on an interval of time dt

$$dW_1 = -k(x_1 - x_2)v_1 dt,$$

generating, as we shall see, a correlation between x_2 and v_1 due to the coupling above. A similar correlation between x_1 and v_2 also appears.

It is straightforward to show that these correlation functions are given by

$$\langle x_1 v_2\rangle = -\frac{\mathcal{D}_1}{\mathcal{D}_2}, \qquad (38)$$

$$\langle x_2 v_1\rangle = -\frac{\mathcal{D}_3}{\mathcal{D}_2}, \qquad (39)$$

where [28]

$$\mathcal{D}_1 = 4\mathcal{N}_{x_1v_2}\mathcal{N}_{x_2x_2}\mathcal{N}_{v_1v_1} - \mathcal{N}_{x_1v_2}\mathcal{N}_{x_2v_1}^2 - 2\mathcal{N}_{x_1x_2}\mathcal{N}_{x_2v_2}\mathcal{N}_{v_1v_1}$$
$$- 2\mathcal{N}_{x_1v_1}\mathcal{N}_{x_2x_2}\mathcal{N}_{v_1v_2} + \mathcal{N}_{x_1v_1}\mathcal{N}_{x_2v_1}\mathcal{N}_{x_2v_2}$$
$$+ \mathcal{N}_{v_1v_2}\mathcal{N}_{x_1x_2}\mathcal{N}_{x_2v_1}, \qquad (40)$$

$$\mathcal{D}_2 = 16\mathcal{N}_{v_2v_2}\mathcal{N}_{x_1x_1}\mathcal{N}_{x_2x_2}\mathcal{N}_{v_1v_1} - 4\mathcal{N}_{v_1v_2}^2\mathcal{N}_{x_1x_1}\mathcal{N}_{x_2x_2}$$
$$- 4\mathcal{N}_{x_1x_1}\mathcal{N}_{x_2v_2}^2\mathcal{N}_{v_1v_1} + 4\mathcal{N}_{v_1v_2}\mathcal{N}_{x_1x_1}\mathcal{N}_{x_2v_1}\mathcal{N}_{x_2v_2}$$
$$- 4\mathcal{N}_{v_2v_2}\mathcal{N}_{x_1x_1}\mathcal{N}_{x_2v_1}^2 - 4\mathcal{N}_{v_2v_2}\mathcal{N}_{x_2x_2}\mathcal{N}_{x_1v_1}^2$$
$$- 4\mathcal{N}_{x_1v_2}^2\mathcal{N}_{x_2x_2}\mathcal{N}_{v_1v_1} + 4\mathcal{N}_{v_1v_2}\mathcal{N}_{x_2x_2}\mathcal{N}_{x_1v_1}\mathcal{N}_{x_1v_2}$$
$$+ \mathcal{N}_{v_1v_2}^2\mathcal{N}_{x_1x_2}^2 + \mathcal{N}_{x_2v_2}^2\mathcal{N}_{x_1v_1}^2 + 4\mathcal{N}_{x_2v_2}\mathcal{N}_{x_1x_2}\mathcal{N}_{x_1v_2}\mathcal{N}_{v_1v_1}$$

$$- 4\mathcal{N}_{v_2 v_2}\mathcal{N}_{v_1 v_1}\mathcal{N}_{x_1 x_2}^2 - 2\mathcal{N}_{v_1 v_2}\mathcal{N}_{x_2 v_2}\mathcal{N}_{x_1 x_2}\mathcal{N}_{x_1 v_1}$$

$$+ \mathcal{N}_{x_1 v_2}^2\mathcal{N}_{x_2 v_1}^2 - 2\mathcal{N}_{v_1 v_2}\mathcal{N}_{x_2 v_1}\mathcal{N}_{x_1 x_2}\mathcal{N}_{x_1 v_2}$$

$$- 2\mathcal{N}_{x_1 v_1}\mathcal{N}_{x_1 v_2}\mathcal{N}_{x_2 v_1}\mathcal{N}_{x_2 v_2} + 4\mathcal{N}_{v_2 v_2}\mathcal{N}_{x_2 v_1}\mathcal{N}_{x_1 x_2}\mathcal{N}_{x_1 v_1},$$

$$(41)$$

$$\mathcal{D}_3 = 4\mathcal{N}_{x_1 x_1}\mathcal{N}_{x_2 v_1}\mathcal{N}_{v_2 v_2} - \mathcal{N}_{x_2 v_1}\mathcal{N}_{x_1 v_2}^2 - 2\mathcal{N}_{x_1 x_2}\mathcal{N}_{x_1 v_1}\mathcal{N}_{v_2 v_2}$$

$$- 2\mathcal{N}_{x_1 x_1}\mathcal{N}_{x_2 v_2}\mathcal{N}_{v_1 v_2} + \mathcal{N}_{x_2 v_2}\mathcal{N}_{x_1 v_1}\mathcal{N}_{x_1 v_2}$$

$$+ \mathcal{N}_{v_1 v_2}\mathcal{N}_{x_1 x_2}\mathcal{N}_{x_1 v_2}.$$

$$(42)$$

Observe that we can swap $\mathcal{D}_1$ and $\mathcal{D}_3$ by the transformation $1 \leftrightarrow 2$.

In the equilibrium limit $T_1 = T_2 = T$, all the terms of the form $\mathcal{N}_{xv}$ will vanish. In consequence, the couplings represented in Eqs. (38) and (39) will also vanish. In equilibrium the flux of heat ceases and velocities decouple from positions, as in the following cases shown below.

C. Interesting limits

Two interesting limits arise. First, by decoupling the particles

$$k = 0 \Rightarrow \mathcal{Q}_{\Delta\Delta} = \mathcal{Q}_{\Lambda\Lambda} = \mathcal{Q}_{\Delta\Delta} = \mathcal{R}_{\Delta\Delta} = \mathcal{H} = 0.$$

The distribution is given by the product of two independent Boltzmann terms:

$$p^{ss}(x_1, x_2, v_1, v_2) = \frac{mk'}{(2\pi)^2 T_1 T_2}$$
$$\times \exp\left\{ -\frac{k' x_1^2}{2T_1} - \frac{mv_1^2}{2T_1} - \frac{k' x_2^2}{2T_2} - \frac{mv_2^2}{2T_2} \right\}.$$

$$(43)$$

Second, by taking the equilibrium (same temperature) case $T_1 = T_2 = T$. The final result corresponds to the Boltzmann distribution:

$$p^{eq}(x_1, x_2, v_1, v_2) = \frac{m\sqrt{k'(k'+2k)}}{(2\pi T)^2}\exp\left\{ -\frac{k' x_1^2}{2T} - \frac{k' x_2^2}{2T} \right.$$
$$\left. -\frac{k(x_1 - x_2)^2}{2T} - \frac{mv_1^2}{2T} - \frac{mv_2^2}{2T} \right\}. \quad (44)$$

V. THERMAL CONDUCTANCE

We are going to obtain the current of energy (heat) between the two Brownian particles by two methods: the exact direct calculation of the work rate between the particles, and a Green-Kubo formalism appropriate for finite systems [18].

The GK formalism [29] has applications for many problems such as fluid slab flow properties [30], diffusion in granular fluids [31–33], fluctuation-dissipation theory [34,35], thermal conductance in condensed-matter systems [36,37], viscosity of trapped Bose gas [38], triple-point bulk and shear viscosities [39,40] or self-diffusion [41] for Lennard-Jones fluids, among others. The GK method de-

pends crucially on the convergence of time integrations of flux-flux correlation functions.

The convergence of the GK integral depends on the flux-flux time-correlation functions decaying fast enough; otherwise the time integration will diverge such as what happens for two-dimensional hydrodynamic systems [42]. This is due to the mode coupling between hydrodynamic modes generating a t^{-1}-dependent tail in the velocity correlations. However, for three dimensions the tail goes as $t^{-3/2}$ [42–44] and the Green-Kubo integral converges. On the other hand, in one dimension, nondiffusive effects can affect the validity of Fourier's law while a Green-Kubo approach might still be valid [45].

A. Energy flux

In order to proceed, we will define the energies and fluxes for our system. The "local" energy density will be given by

$$\epsilon_{1,2} = \frac{1}{2}mv_{1,2}^2 + \frac{1}{2}k' x_{1,2}^2. \quad (45)$$

The contact of the particles with the thermal reservoirs and the presence of the dissipative terms imply a flux of energy into, and out of, the system at both positions. These instantaneous contact fluxes are given by [17]:

$$j_{c1} = -\gamma v_1^2 + v_1 \eta_1, \quad (46)$$

$$j_{c2} = -\gamma v_2^2 + v_2 \eta_2. \quad (47)$$

As the coupling spring acts as the interaction channel between the particles, we define, for each particle, the transmitted heat flux (energy/time) as

$$j_{t1} = -k[x_1(t) - x_2(t)]v_1, \quad (48)$$

$$j_{t2} = -k[x_2(t) - x_1(t)]v_2. \quad (49)$$

The local interparticle elastic energy is defined as

$$E_{el} = \frac{1}{2}k[x_1(t) - x_2(t)]^2. \quad (50)$$

The total balance of energy requires that the excess energy be stored in the spring potential. Thus, it is straightforward to see that the above definitions do respect energy balance since

$$j_{t1} + j_{t2} = -dE_{el}/dt.$$

The effective transfer flux j_{12} can now be defined:

$$j_{12} = \frac{1}{2}(j_{t1} - j_{t2}) = -k[x_1(t) - x_2(t)]\left(\frac{v_1(t) + v_2(t)}{2} \right).$$

$$(51)$$

The definition above corresponds to sharing the elastic energy, defined in Eq. (59), in equal parts between the neighboring particles.

B. Direct calculation of κ

The thermal conductance is

$$\kappa \equiv \kappa(T, \Delta T) = \frac{\partial}{\partial \Delta T} \langle j_{12} \rangle_{\Delta T}, \qquad (52)$$

where $A_1 = A_2 = 0$, $T_1 = T$, $T_2 = T + \Delta T$, and $\langle \ \rangle_{\Delta T}$ is the average at $\Delta T > 0$. The above expression for κ goes beyond first-order approximation since it contains all the information needed to calculate the heat flux, as shown in

$$\langle j_{12} \rangle_{\Delta T} \equiv \langle j_{12} \rangle(T, \Delta T) = \int_0^{\Delta T} dt \, \kappa(T, t). \qquad (53)$$

The average heat flux is given by $\langle j_{12} \rangle_{\Delta T}$ and can be calculated exactly:

$$\langle j_{12} \rangle_{\Delta T} = -k \left\langle (x_1 - x_2) \left(\frac{v_1 + v_2}{2} \right) \right\rangle = -\frac{k}{2} (\langle x_1 v_2 \rangle - \langle x_2 v_1 \rangle). \qquad (54)$$

Using Eqs. (38) and (39), we write

$$\langle j_{12} \rangle_{\Delta T} = -\frac{k(\mathcal{D}_1 - \mathcal{D}_3)}{2\mathcal{D}_2}, \qquad (55)$$

where the values of $(\mathcal{D}_1, \mathcal{D}_2, \mathcal{D}_3)$ are given in Eqs. (40)–(42).

After some tedious (but straightforward) algebra, the final result is rather simple [28]:

$$\langle j_{12} \rangle_{\Delta T} = 2k\mathcal{H}\Delta T \Rightarrow \kappa = \frac{k^2 \gamma}{2[mk^2 + \gamma^2(k + k')]}, \qquad (56)$$

where κ is exact and independent of T and ΔT.

It is not unexpected to find the flux proportional to ΔT since this result has been obtained for similar models before [2,3,5]. However, Eq. (56) represents the time average over the full dynamics of the system. We do not make any use of approximate master-equation-type methods, such as the Fokker-Planck equation [12], to obtain the value of κ. Our method is equivalent to solving exactly the dynamical equations of motion given the realization of the noise, then taking the noise average, and finally time averaging the final result. In principle, the present approach can be generalized for any type of noise, not only white noise. It is interesting to com-

pare Eq. (56) with the results obtained from a Green-Kubo integration. This will be an interesting test on the validity of the choice of the thermal current, and also of the approximations used in order to derive the Green-Kubo formalism.

C. Green-Kubo calculation of κ

The exact expression for κ above can be compared with proposals in the literature where Green-Kubo formulations for the thermal conductance are given. In the spirit of the previous paragraph, the effective flux $\bar{j}$ plays the role of the fluctuating flux j_{12} for a Green-Kubo relation proposed [18] for obtaining the thermal conductance:

$$\kappa = \lim_{\Delta T \to 0} \frac{\langle \bar{j} \rangle_{\Delta T}}{\Delta T} = \frac{1}{T^2} \int_0^\infty dt \langle \bar{j}(t)\bar{j}(0) \rangle, \qquad (57)$$

where $\langle \ \rangle$ stands for the equilibrium average ($\Delta T = 0$). We write

$$\kappa = \lim_{\Omega \to \infty} \frac{1}{\Omega} \int_0^\Omega dt \frac{1}{(T)^2} \int_0^\infty d\tau \langle j_{12}(t + \tau) j_{12}(t) \rangle_{\Delta T = 0},$$

$$= \lim_{z \to 0^+} \lim_{\theta \to 0^+} \frac{z}{(T)^2} \int_0^\infty dt e^{-zt} \int_0^\infty d\tau e^{-\theta\tau} \langle j_{12}(t + \tau) j_{12}(t) \rangle_{\Delta T = 0}. \qquad (58)$$

Replacing the flux above into Eq. (58), we obtain the Green-Kubo expression for κ:

$$\kappa = \lim_{z \to 0^+} \lim_{\theta \to 0^+} z \int_0^\infty dt e^{-zt} \frac{k^2}{T^2} \int_0^\infty d\tau e^{-\theta\tau}$$
$$\times \left\langle \left[[x_1(t + \tau) - x_2(t + \tau)] \left(\frac{v_1(t + \tau) + v_2(t + \tau)}{2} \right) \right] \right.$$
$$\left. \times \left[[x_1(t) - x_2(t)] \left(\frac{v_1(t) + v_2(t)}{2} \right) \right] \right\rangle_{\Delta T = 0}. \qquad (59)$$

After some algebraic manipulation the expression for the thermal conductance becomes [28]

$$\kappa = \lim_{z \to 0^+} \lim_{\theta \to 0^+} \lim_{\epsilon \to 0^+} \frac{k^2}{16T^2} \int_{-\infty}^\infty \frac{dq_1}{2\pi} \int_{-\infty}^\infty \frac{dq_2}{2\pi} \int_{-\infty}^\infty \frac{dq_3}{2\pi} \int_{-\infty}^\infty \frac{dq_4}{2\pi} \frac{z}{z - [(iq_1 + \epsilon) + (iq_2 + \epsilon) + (iq_3 + \epsilon) + (iq_4 + \epsilon)]}$$

$$\times \frac{(iq_3 + \epsilon)(iq_4 + \epsilon)}{\theta - [(iq_1 + \epsilon) + (iq_3 + \epsilon)]} \langle \{[\tilde{x}_1(iq_1 + \epsilon) - \tilde{x}_2(iq_1 + \epsilon)][\tilde{x}_1(iq_3 + \epsilon) + \tilde{x}_2(iq_3 + \epsilon)]\}$$

$$\times \{[\tilde{x}_1(iq_2 + \epsilon) - \tilde{x}_2(iq_2 + \epsilon)][\tilde{x}_1(iq_4 + \epsilon) + \tilde{x}_2(iq_4 + \epsilon)]\} \rangle$$

$$= \lim_{\theta \to 0^+} \lim_{\epsilon \to 0^+} \frac{k^2 \gamma^2}{4} \int_{-\infty}^\infty \frac{dq_1}{2\pi} \int_{-\infty}^\infty \frac{dq_3}{2\pi} \frac{(iq_3 + \epsilon)(-iq_3 - \epsilon)}{\theta - [(iq_1 + \epsilon) + (iq_3 + \epsilon)]} \frac{1}{[\Gamma(iq_1 + \epsilon) + k][\Gamma(-iq_1 - \epsilon) + k][\Gamma(iq_3 + \epsilon) - k][\Gamma(-iq_3 - \epsilon) - k]},$$
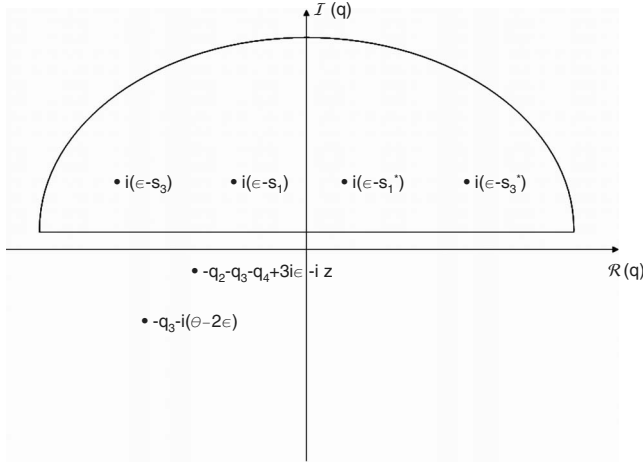
$$(60)$$

FIG. 2. Integration path over the poles for the Green-Kubo calculation of the conductance.

where the poles are given by

$$s_1 = -\frac{\gamma}{2m} + i \sqrt{\frac{k'}{m} - \frac{\gamma^2}{4m^2}};$$

$$s_3 = -\frac{\gamma}{2m} + i \sqrt{\frac{(2k + k')}{m} - \frac{\gamma^2}{4m^2}},$$

and the integration path is shown in Fig. 2.

Equation (60) gives exactly the same result of Eq. (56), showing that both approaches are completely consistent.

D. Discussion

The coherence shown for the thermal conductance results for finite systems, calculated either directly, Eq. (56), or via the Green-Kubo approach, Eq. (58), seems to point to the validity of considering the microscopic work as the correct fluctuating flux variable to be used for coupled particle systems. In fact, for more realistic models in which the number of particles is large, solving the same problem for nonharmonic potentials might be the way to obtain a rigorous demonstration of Fourier's law.

In our case, despite the somewhat involved aspects of the algebra, the final value for κ is quite simple and carries the influence of both couplings, k and k', the friction coefficient γ, and the inertia m. The program we followed in order to find κ is equivalent to solving the exact equations of motion of the Brownian particles system for each realization of the noise functions, and then taking the average over the noise. No approximations of any sort are necessary once the basic model is provided. The present treatment can be extended to other distinct kinds of noise, such as colored noise (non-Markovian), or even distinct heat baths acting on the same particles.

However, the present method can readily be extended to (finite) systems composed of more than two Brownian par-

ticles, systems that may be large enough to be taken as "macroscopic." The difficulties to treat such systems are operational or numerical rather than conceptual.

VI. CONCLUSIONS

Brownian particles (BP) are an excellent laboratory for studying nonequilibrium physics. They are simple to describe but present many of the features of more complex models, such as the possibility of reaching stationary states when submitted to thermal contacts at distinct temperature. They are also good approximations for larger systems, such as polymers, which could be modeled by chains of BP attached to each other by some type of attractive potential.

Another interesting characteristic of such systems is that they are simple enough so that we can extract exact solutions for their long-time behavior. This allows us to obtain results that are hard to come by using other methods. It is already known that we can obtain exactly the equilibrium probability distribution for Brownian particles subjected to Markovian or non-Markovian noise, or a combination of both. This type of external forcing allows us to keep a system formed by a single particle constantly on an out of equilibrium steady-state.

Furthermore, techniques based on time averaging are very interesting since they are ensemble independent, driven only by the dynamical relations governing the interaction Brownian particle-heat bath. In fact, this corresponds to following a system during the realization of an experiment.

In the present work, we have studied the thermal conductance for a system of coupled particles, by taking advantage of the mechanically simple characteristics of Brownian particles and of time averaging. Our system consists of two particles coupled by a spring potential, with the heat flux flow j_{12} being due to the mechanical work done through the spring coupling the two particles. The particles may be kept in contact with distinct thermal baths and the flow of energy may be obtained by means of the thermal conductance coefficient κ, appropriate for small systems. The latter is calculated both from first principles, and by means of a Green-Kubo formulation, and the obtained exact results are identical. The final form of κ depends only on the variables of the system, such as the mass of the particles, the spring couplings and the friction coefficients. The thermal conductance can be thought as a first step for obtaining the equivalent form for more sophisticated macroscopic systems such as long polymers.

We believe that the coherence between the exact direct calculation and the exact Green-Kubo formulation for κ shows the correctness of the basic definitions especially that of the heat flux, used in the problem.

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