

Microscopic theory of nonisothermal Brownian motion

Alec Maassen van den Brink^{1,*} and H. Dekker^{1,2}

¹*Institute for Theoretical Physics, University of Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands*
and *Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong*[†]

²*TNO Physics and Electronics Laboratory, P.O. Box 96864, 2509 JG Den Haag, The Netherlands*

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We present the statistical mechanical derivation of the Fokker-Planck equation for nonisothermal stochastic processes. The analysis proceeds by applying nonlinear-process projection methods to a mesoscopic system coupled to a heat bath. Our result provides a microscopic foundation for the phenomenological theory [H. Dekker, Phys. Rev. A **43**, 4224 (1991)] and generalizes the canonical Kramers model. [S1063-651X(97)00605-3]

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I. INTRODUCTION

Nonisothermal Brownian motion is a stochastic process in which, besides position and momentum, the (local) temperature is among the fluctuating variables. Since both momentum and thermal fluctuations are most prominent for small physical dimensions, such a process is a logical extension of the theory of Brownian motion to mesoscopic systems with small heat capacitance, where energy density rather than local temperature is the conserved slow variable. A phenomenological analysis was first given by one of us in Refs. [1,2]. Using fluctuation-dissipation arguments, mechanical and thermal noise were added to the deterministic evolution equations such that the total Fokker-Planck operator supposedly possessed the known equilibrium distribution—involving the availability [3]—as its stationary solution. Various limiting cases and approximations of the formalism were presented and applied to lifetime calculation problems in Josephson devices. In the thermally isolated case the results showed a substantial barrier (and, therefore, lifetime) enhancement.

In this paper we give a microscopic derivation of nonisothermal Brownian motion. We concentrate on establishing the general equations rather than on specific cases. The analysis proceeds by means of nonlinear-process (i.e., suitable for nonlinear fluctuations) projectors, as outlined in Sec. II. By weakly coupling a mesoscopic system (e.g., a superconducting quantum interference device) to a heat bath, its microcanonically fixed energy E becomes a random variable (along with x and p), yielding the general nonlinear stochastic process in Sec. III. Upon introducing a novel mean force term (different from the free energy gradient) a Fokker-Planck equation (FPE) modeling as in [1,2] is reconciled with ensemble theory—while originally starting from an incorrect equilibrium distribution, cf. Sec. IV—even slightly beyond its initial scope (viz., to nonconstant transport coefficients). Some final remarks are made in Sec. IV. An exhaustive account of the theory can be found in Ref. [4].

II. NONLINEAR-PROCESS PROJECTORS

Consider a classical dynamical system with Hamiltonian H , the microscopic state being represented by a point Γ in its phase space Π . The time evolution of gross variables $a = \{a_i\}$ —defined microscopically as phase space functions $a = A(\Gamma)$ —is stochastic since, for an initial macrostate a , the microstate is only constrained to $S(a) \equiv \{\Gamma | A(\Gamma) = a\}$. Parametrizing each such hypersurface by coordinates Ω_a [so that $\Gamma = (a, \Omega_a)$ and $d\Gamma = da d\Omega_a$], it is possible to average over the initial value of Ω_a once the initial probability density on $S(a)$ is known. We suppose the system to have an equilibrium distribution $\bar{\rho}(\Gamma)$, i.e., $\mathcal{L}\bar{\rho}(\Gamma) \equiv \{H(\Gamma), \bar{\rho}(\Gamma)\} = 0$ (\mathcal{L} is the Liouville operator), and take the initial distribution $\rho(\Gamma, 0)$ from the stationary preparation class: $\rho(\Gamma, 0) = P(a, 0) \bar{w}(a, \Omega_a)$, with the stationary conditional density $\bar{w}(a, \Omega_a) = \bar{\rho} / \int d\Omega_a \bar{\rho}$.

Given an ensemble of systems, all in the macrostate a , one can introduce the reversible drift $v(a) = \int d\Omega_a \bar{w}(a, \Omega_a) \dot{A}(a, \Omega_a)$, with $\dot{A} = -\mathcal{L}A$. However, the individual members in general evolve with velocity $\dot{A}(a, \Omega_a) \neq v(a)$ and also $\int d\Omega_a w(a, \Omega_a, t) \dot{A}(a, \Omega_a) \neq v(a)$, since $w(a, \Omega_a, t)$ typically differs from \bar{w} even if the ensemble is the subset with $A(\Gamma) = a$ of a larger one from the stationary preparation class. In addition to the drift v there thus is a diffusive current, as will be seen in the projection operator formalism [5,6].

The set of all phase space functions is made into a Hilbert space \mathcal{H} by introducing the inner product

$$\langle X, Y \rangle = \int d\Gamma \bar{w}(\Gamma) X(\Gamma) Y(\Gamma). \quad (1)$$

One then defines the projector

$$(\mathcal{P}X)(\Gamma) = \int da \Psi^a(\Gamma) \langle \Psi^a, X \rangle, \quad (2)$$

with $\Psi^a(\Gamma) = \delta(A(\Gamma) - a)$, which allows decomposition of the evolution operator into a “drift,” a “dissipative,” and a “noise” part as

*Electronic address: alec@phy.cuhk.edu.hk

[†]Present address.

$$e^{-\mathcal{L}t} = e^{-\mathcal{L}t} \mathcal{P} - \int_0^t ds e^{\mathcal{L}(s-t)} \mathcal{P} \mathcal{L} \mathcal{Q} e^{-\hat{\mathcal{L}}s} \mathcal{Q} + \mathcal{Q} e^{-\hat{\mathcal{L}}t} \mathcal{Q}, \quad (3)$$

where $\mathcal{Q} = 1 - \mathcal{P}$, $\hat{\mathcal{L}} = \mathcal{Q} \mathcal{L} \mathcal{Q}$.

Given an initial distribution from the stationary preparation class, and with $\rho(\Gamma, t) = e^{\mathcal{L}t} \rho(\Gamma, 0)$, the evolution of the macroscopic distribution $P(a, t) = \int d\Gamma \Psi^a(\Gamma) \rho(\Gamma, t)$ obeys

$$\begin{aligned} \partial_t P(a, t) = & -\partial_{a_i} [v_i(a) P(a, t)] + \int_0^t ds \partial_{a_i} \int da' D_{ij}(a, a', s) \\ & \times \bar{P}(a') \partial_{a_j} \frac{P(a', t-s)}{\bar{P}(a')}, \end{aligned} \quad (4)$$

with

$$v_i(a) = \langle \Psi^a \dot{A}_i \rangle, \quad (5)$$

$$D_{ij}(a, a', s) = \langle \Psi^{a'} \dot{A}_j, \mathcal{Q} e^{-\hat{\mathcal{L}}s} \mathcal{Q} \Psi^a \dot{A}_i \rangle \quad (6)$$

for the drift and diffusion kernels, respectively.

Equation (4) is still exact, and approximations must be introduced. Following Refs. [1,2] we are interested in the Markovian limit (ML), wherein the kernels (6) rapidly decay to zero so that $P(a, t)$ can be taken outside both s and a' integrals. This yields the FPE

$$\begin{aligned} \partial_t P(a, t) = & -\partial_{a_i} [v_i(a) P(a, t)] \\ & + \partial_{a_i} [K_{ij}(a) \bar{P}(a) \partial_{a_j} (\bar{P}(a)^{-1} P(a, t))], \end{aligned} \quad (7)$$

with

$$\begin{aligned} K_{ij}(a) = & \int_0^\infty ds \int da' D_{ij}(a, a', s) \\ = & \langle \dot{A}_j, \mathcal{Q} \hat{\mathcal{L}}^{-1} \mathcal{Q} \Psi^a \dot{A}_i \rangle, \end{aligned} \quad (8)$$

where the last line follows from Eq. (6). Since $\hat{\mathcal{L}}$ has the null space \mathcal{PH} , $\hat{\mathcal{L}}^{-1}$ is defined only in \mathcal{QH} and only in that subspace will this notation be used. With Eq. (5) for $v(a)$ one has $\partial_{a_i} [v_i(a) \bar{P}(a)] = 0$ [5], so that \bar{P} is an exact stationary solution of the approximate Eq. (7).

III. NONISOTHERMAL KRAMERS EQUATION

We write $\Gamma_i = (\Gamma_0, \Gamma_b)$ for the coordinates of ‘‘system plus bath,’’ wherein $\Gamma_0 = (x_0, p_0, \Gamma_1)$ with $\Gamma_1 = (x_i, p_i)_{i \geq 1}$. The Hamiltonian is taken to be

$$H_i(\Gamma_i) = H_0(\Gamma_0) + H_b(\Gamma_b) + H_1(\{x_i\}, \{x_{b,j}\}), \quad (9)$$

where

$$H_0(\Gamma_0) = \sum_{i \geq 0} \frac{p_i^2}{2m_i} + \Phi(\{x_{ij}\}), \quad (10)$$

yielding

$$\mathcal{L}_0 = \frac{\partial \Phi(\{x_{ij}\})}{\partial x_j} \partial_{p_j} - \frac{p_j}{m_j} \partial_{x_j}. \quad (11)$$

The bath is taken to be infinite, so that the canonical ensemble will be used for the total system, i.e., the microscopic equilibrium density reads

$$\bar{\rho}_i(\Gamma_i) = Z_i^{-1} e^{-\beta_i H_i(\Gamma_i)}, \quad (12)$$

where

$$Z_i = \int d\Gamma_i e^{-\beta_i H_i(\Gamma_i)}, \quad (13)$$

with β_i the inverse reservoir temperature. To derive a Brownian thermodynamics, we define the observables as $a = (x, p, E) = (x_0, p_0, H_0(\Gamma_0))$. This choice is appropriate if $m = m_0 \gg m_{i \geq 1}$, so that the 0 particle is much slower than the other ones. The coupling H_1 is taken infinitesimal—only then a picture of the total system as ‘‘matrix plus reservoir’’ (Fig. 1 of Refs. [1,2]) is meaningful. This leads to $Z_i \approx Z_0 Z_b$; for the equilibrium macrodistribution it implies

$$\begin{aligned} \bar{P}(x, p, E) = & \frac{e^{-\beta_r E}}{Z_0} \int d\Gamma_1 \delta(H_0(\Gamma_0) - E) \\ = & \exp\{\mathcal{S}_m(x, p, E) + \beta_r [F_0(\beta_r) - E]\} \\ = & \exp\{\beta_r [F_0(\beta_r) - \mathcal{A}_m(x, p, E, \beta_r)]\}, \end{aligned} \quad (14)$$

with the microcanonical availability [3,7] defined by

$$\begin{aligned} \mathcal{A}_m(x, p, E) = & E - T_r \mathcal{S}_m(x, p, E) \\ = & \mathcal{F}_m(x, p, E) + (T(x, p, E) - T_r) \mathcal{S}_m(x, p, E), \end{aligned} \quad (15)$$

where

$$\mathcal{S}_m(x, p, E) = \ln \int d\Gamma_1 \delta(H_0(x, p, \Gamma_1) - E) \quad (16)$$

is the conditional entropy, $T^{-1} = \partial_E \mathcal{S}_m(x, p, E)$, and $\mathcal{F}_m = E - T \mathcal{S}_m$, while $F_0 = -T_r \ln Z_0$ is the unconditional free energy.

To lowest (i.e., zeroth) order in H_1 , the (x, p) dynamics at a given point (x', p', E') in macroscopic state space coincides with the microcanonical one. Hence, both the drifts $v_i(x', p', E')$ and the diffusion tensor $K_{ij}(x', p', E')$ (with $i, j = x, p$) are calculated in the ensemble with $\bar{\rho}_m(\Gamma_0) = Z_m^{-1} \delta(H_0(\Gamma_0) - E')$. In particular, $v_p = f$ with

$$f(x, p, E) = e^{-S_m(x, p, E)} \partial_x \int_{-\infty}^E dE' e^{S_m(x, p, E')} \quad (17)$$

while $v_x = p/m$. For the evolution of E itself the coupling H_1 must be considered. From Eq. (5) one obtains $v_E = \langle \Psi^a, \dot{H}_0 \rangle = 0$ for the energy drift by time reversal symmetry. Taking the ML also for the E diffusion, we arrive at the nonisothermal FPE

$$\partial_t P(x,p,E,t) = \left[-\frac{p}{m} \partial_x + \partial_p \{ -f + K e^{\mathcal{S}_m} \partial_p e^{-\mathcal{S}_m} \} \right. \\ \left. + \partial_E M e^{-\beta_r A_m} \partial_E e^{\beta_r A_m} \right] P(x,p,E,t) \quad (18)$$

with $K_{pp} = K$ (other K_{ij} are zero, for $\dot{Q} = 0$), viz.,

$$K(x,p,E) = \langle \partial_{x_0} \Phi + f(x,p,E), \hat{\mathcal{L}}_t^{-1} \delta(x_0 - x) \delta(p_0 - p) \\ \times \delta(H_0(\Gamma_0) - E) (\partial_{x_0} \Phi + f(x,p,E)) \rangle \quad (19)$$

and with the energy diffusion coefficient

$$M(x,p,E) = \langle \dot{H}_0, \hat{\mathcal{L}}_t^{-1} \delta(x_0 - x) \delta(p_0 - p) \\ \times \delta(H_0(\Gamma_0) - E) \dot{H}_0 \rangle. \quad (20)$$

IV. FINAL REMARKS

Rewriting the momentum diffusion term in Eq. (18) as

$$\partial_p K e^{\mathcal{S}_m} \partial_p e^{-\mathcal{S}_m} = \partial_p \frac{K}{mT} (p + mT \partial_p), \quad (21)$$

the friction coefficient may be identified as $2\lambda = K/mT$ [1,2]. However, the effective λ in the Smoluchowski limit in general acquires both position and temperature dependence even if taken constant in Eq. (18). Similarly, the heat diffusion term allows the introduction of $\kappa = M/T T_r$ as the heat conductance. Equation (18) may also serve as a starting point for further approximations, studying concrete models (e.g., to calculate lifetimes of metastable states), etc., without evaluating microscopic expressions as

(19) or (20), which, however, do restrict the freedom to model the various coefficients [4]. For example, only M can have an additional dependence on T_r , while f is entirely fixed by \mathcal{S}_m ; see Eq. (17).

The present microscopic theory is a ‘‘necessarily modest contribution’’ (Ref. [2], Sec. 5). For example, quantum effects are not incorporated. Hence, the study of macroscopic quantum tunneling [8–10] in the nonisothermal regime, or the justification of Eq. (18) when the functions $\{f, \mathcal{S}_m, K, M\}$ cannot be calculated in the classical approximation, is still beyond reach. The latter will, e.g., be relevant to superconductivity, but quantum features will show up at low temperatures also in other systems. While at low T the present results satisfy the minimal requirement of being well defined ($\mathcal{T} = 0$ constitutes a natural boundary in Eq. (18); see Ref. [4]) our analysis should be carried further to the quantum case *à la* Caldeira and Leggett [9].

Our derivation of Eq. (18) generalizes the formulas of Refs. [1,2] to position and temperature dependent transport coefficients. By founding our analysis on statistical mechanics we have ensured that the results are compatible with classical equilibrium statistics. This solves a problem with Ref. [2], where the stationary measure is taken as $\bar{P} \propto \exp\{-\beta_r A\} dx dp dS$ instead of the correct $\bar{P} \propto \exp\{-\beta_r A_m\} dx dp dE$ [see Eq. (14)], the difference being nontrivial for genuine nonlinear fluctuations.

In conclusion, the present work connects the theory of nonisothermal stochastic processes to conventional statistical mechanics.

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