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Quantum description of Einstein's Brownian motion

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A fully quantum treatment of Einstein's Brownian motion is given, stressing in particular the role played by the two original requirements of translational invariance and connection between dynamics of the Brownian particle and atomic nature of the medium. The former leads to a clearcut relationship with a generator of translation-covariant quantum-dynamical semigroups recently characterized by Holevo, the latter to a formulation of the fluctuation-dissipation theorem in terms of the dynamic structure factor, a two-point correlation function introduced in seminal work by Van Hove, directly related to density fluctuations in the medium and therefore to its atomistic, discrete nature. A microphysical expression for the generally temperature dependent friction coefficient is given in terms of the dynamic structure factor and of the interaction potential describing the single collisions. A comparison with the Caldeira-Leggett model is drawn, especially in view of the requirement of translational invariance, further characterizing general structures of reduced dynamics arising in the presence of symmetry under translations.

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I. INTRODUCTION

A century has passed since Einstein published the first of a series of papers on the theory of Brownian movement [1,2], a pioneering work attempting to provide a suitable theoretical framework for the description of a long-standing experimental puzzle [3]. Einstein's investigation went much beyond the explanation of an interesting experiment, proving a milestone in the understanding of statistical mechanics of nonequilibrium processes, motivating and inspiring physical and mathematical research on stochastic processes. By now the term Brownian motion is ubiquitously found in the physical literature, at both the quantum and classical levels, used as a kind of keyword in a wealth of situations relying on a description in terms of mathematical structures or physical concepts akin to those first appearing in the explanation of Einstein's Brownian motion. In this paper we address the question of a proper quantum description of Brownian motion in the sense of Einstein, i.e., the motion of a massive test particle in a homogeneous fluid made up of much lighter particles. In doing so we actually go back to Einstein's real motivation in examining Brownian motion, i.e., to demonstrate the molecular, discrete nature of matter. His aim was in fact to give a decisive argument probing the correctness of the molecular-kinetic conception of heat, a question he considered most important, as stressed in the very last sentence of the paper, actually quite emphatic in the original German version: "Möge es bald einem Forscher gelingen, die hier aufgeworfene, für die Theorie der Wärme wichtige Frage zu entscheiden!" [4].

In contrast with previous approaches and results, based either on a modeling of the environment aiming at exact solubility given a certain phenomenological ansatz [5], or on an axiomatic approach relying on mathematical input [6,7], or on the exploitation of semiclassical correspondence [8], we will base our microscopic analysis on the two key features of Einstein's Brownian motion: homogeneity of the background medium, reflected in the property of translational invariance, and the atomic nature of matter responsible for density fluctuations, showing up in a suitable formulation of the fluctuation-dissipation relationship. Translational invariance comes about because of the homogeneity of the fluid and the translational invariance of the interaction potential between test particle and elementary constituents of the fluid. This fundamental symmetry property leads to important restrictions both on the expression for possible interactions and on the structure of the completely positive generator of a quantum-dynamical semigroup describing the Markovian reduced dynamics. The first key point is therefore to consider the proper type of translational-invariant interaction leading to Einstein's Brownian motion, thus fixing the relevant correlation function appearing in the structure of the generator of the dynamics, which turns out to be the so-called dynamic structure factor and provides the natural formulation of the fluctuation-dissipation relationship for the case of interest first put forward by Van Hove in an epochal paper [9]. Given that the dynamics can be fairly assumed to be Markovian, the second key point is the characterization of the structure of generators of quantum-dynamical semigroups covariant under a suitable symmetry group, in this case $\mathbb{R}$, i.e., translations, which has been recently given in most relevant work by Holevo [10].

The present paper partially builds on previous work [11–13], putting it in a wider conceptual and theoretical framework, providing the previously unexplored connection to the fluctuation-dissipation theorem and a general microphysical expression for the friction coefficient in terms of a suitable autocorrelation function. This kinetic approach to

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quantum dissipation is further compared with the one by Caldeira and Leggett, also in view of recent criticism on the realm of validity of the last approach [14,15], showing how the Caldeira-Leggett model is recovered as the long-wavelength limit of this kinetic approach. In this way a different approach to the quantum description of decoherence and dissipation is put forward, which, though obviously not universally valid, could provide a direct connection between a precise microphysical model and reduced dynamics for a wide class of open quantum systems, characterized by suitable symmetries. While universality might often be a loose word in such a complex framework, this precise microphysical modeling makes a close, quantitative comparison between present [16–19] and next generation experiments on decoherence and dissipation in principle feasible.

The paper is organized as follows: In Sec. II we introduce the basic possible translationally invariant interactions, putting into evidence their effect on the structure of the reduced dynamics, also in comparison with previous models in the literature. In Sec. III we point out the relevant interaction for the description of Einstein's quantum Brownian motion, showing the related expression of the fluctuation-dissipation theorem. In Sec. IV we come to the formulation of Einstein's quantum Brownian motion putting into evidence the general microphysical expression for the friction coefficient in terms of a suitable autocorrelation function. In Sec. V we finally comment on our results and discuss possible future developments.

II. TRANSLATIONAL INVARIANCE

As a first step we characterize the general structure of microscopic Hamiltonians leading to a translationally invariant reduced dynamics for the test particle. Due to translational invariance the test particle has to be free apart from the interaction with the fluid, subject at most to a potential linearly depending on position, e.g., a constant gravitational field, so that in particular it has a continuous spectrum. The fluid is supposed to be stationary and homogeneous, and for simplicity, without loss of generality, possessing inversion symmetry, so that energy, momentum, and parity are constants of the motion.

A. Translationally invariant interactions

1. Characterization of translationally invariant interactions

The microscopic Hamiltonian may be written in the form

$$H_{\mathrm{PM}} = H_{\mathrm{P}} + H_{\mathrm{M}} + V_{\mathrm{PM}}, \tag{1}$$

where the subscripts P and M stand for particle and matter respectively, while H_{P} and H_{M} satisfy the aforementioned constraints. The key point is the characterization of a suitable translationally invariant interaction potential, which we put forward in the formalism of second quantization. This nonrelativistic field theoretical approach is the natural one in order to account for statistics and more generally many-particle features of the background macroscopic system, also proving useful in microphysical calculations [20] and allowing us to deal not only with the one-particle sector of the Fock space in which the fields referring to the test particle are described. The interaction potential between test particle and matter will have the general form

$$V_{\mathrm{PM}} = \int d^3\boldsymbol{x} \int d^3\boldsymbol{y}\, A_{\mathrm{P}}(\boldsymbol{x}) t(\boldsymbol{x}-\boldsymbol{y}) A_{\mathrm{M}}(\boldsymbol{y}), \tag{2}$$

where $t(\boldsymbol{x})$ is a $\mathbb{C}$-number, in the following applications short-range, interaction potential; $A_{\mathrm{P}}(\boldsymbol{x})$ and $A_{\mathrm{M}}(\boldsymbol{y})$ are self-adjoint operators built in terms of the fields

$$\varphi_{\mathrm{P}}(\boldsymbol{x}) = \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^{3/2}} e^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{x}} a_{\boldsymbol{p}} \quad \text{and}$$

$$\varphi_{\mathrm{M}}(\boldsymbol{y}) = \int \frac{d^3\boldsymbol{\eta}}{(2\pi\hbar)^{3/2}} e^{(i/\hbar)\boldsymbol{\eta}\cdot\boldsymbol{y}} b_{\boldsymbol{\eta}}, \tag{3}$$

respectively, satisfying canonical commutation or anticommutation relations. Equation (2) can be most meaningfully rewritten in terms of the Fourier transform of the interaction potential

$$\tilde{t}(\boldsymbol{q}) = \int \frac{d^3\boldsymbol{x}}{(2\pi\hbar)^3} e^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{x}} t(\boldsymbol{x}), \tag{4}$$

where the continuous parameter $\boldsymbol{q}$, to be seen as a momentum transfer, has a natural group theoretical meaning as the label of the irreducible unitary representations of the group of translations, as to be stressed later on, thus coming to the equivalent expression

$$V_{\mathrm{PM}} = \int d^3\boldsymbol{q}\, \tilde{t}(\boldsymbol{q}) A_{\mathrm{P}}(\boldsymbol{q}) A_{\mathrm{M}}^{\dagger}(\boldsymbol{q}), \tag{5}$$

where the operators $A_{\mathrm{P}}(\boldsymbol{q})$ and $A_{\mathrm{M}}(\boldsymbol{q})$ are defined according to

$$A_{\mathrm{P/M}}(\boldsymbol{q}) = \int d^3\boldsymbol{x} e^{-(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{x}} A_{\mathrm{P/M}}(\boldsymbol{x}). \tag{6}$$

Translational invariance of the interaction, leading to the invariance of V_{PM} under a global translation, is obvious in Eq. (2) because the coupling through the potential depends only on the relative positions of the two local operator densities, and comes about in Eq. (5) because the operators in Eq. (6) simply transform by a phase $\exp[(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{a}]$ under a translation of step $\boldsymbol{a}$.

We will now consider two general types of physically meaningful translationally invariant couplings, corresponding to quite distinct situations. The first is a density-density coupling, which as argued in the next sections is the one relevant for the quantum description of Einstein's Brownian motion, given by the identifications

$$A_{\mathrm{P/M}}(\boldsymbol{x}) = \varphi_{\mathrm{P/M}}^{\dagger}(\boldsymbol{x}) \varphi_{\mathrm{P/M}}(\boldsymbol{x}) \equiv N_{\mathrm{P/M}}(\boldsymbol{x}), \tag{7}$$

which, introducing the $\boldsymbol{q}$ component of the number-density operator $\rho_{\boldsymbol{q}}$ [21,22]

$$\rho_{\boldsymbol{q}} \equiv \int d^3\boldsymbol{x}\, e^{-(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{x}} N_{\mathrm{M}}(\boldsymbol{x}) = \int \frac{d^3\eta}{(2\pi\hbar)^3} b_{\boldsymbol{\eta}}^{\dagger} b_{\boldsymbol{\eta}+\boldsymbol{q}}, \tag{8}$$

can be written

$$V_{\rm PM} = \int d^3\boldsymbol{q}\, \tilde{t}(\boldsymbol{q}) A_{\rm P}(\boldsymbol{q}) \rho^{\dagger}_{\boldsymbol{q}}(\boldsymbol{q}). \tag{9}$$

Note that an interaction of the form (9), besides being translationally invariant, commutes with the number operators $N_{\rm P}$ and $N_{\rm M}$, so that the elementary interaction events do bring in exchanges of momentum between the test particle and the environment, but the number of particles or quanta in both systems is independently conserved, thus typically describing an interaction in terms of collisions.

The other type of interaction we shall consider is a density-displacement coupling, corresponding to the expressions $A_{\rm P}(\boldsymbol{x}) = N_{\rm P}(\boldsymbol{x})$, as above for the particle, and

$$A_{\rm M}(\boldsymbol{x}) = \int \frac{d^3\boldsymbol{\eta}}{(2\pi\hbar)^3}(b_{\boldsymbol{\eta}} + b^{\dagger}_{-\boldsymbol{\eta}}) e^{(i/\hbar)\boldsymbol{\eta}\cdot\boldsymbol{x}} \equiv u(\boldsymbol{x}) \tag{10}$$

for the macroscopic system, where $u(\boldsymbol{x})$ is often called the displacement operator [23,24], thus leading in terms of the Fourier transformed quantities to

$$V_{\rm PM} = \int d^3\boldsymbol{q}\, \tilde{t}(\boldsymbol{q}) A_{\rm P}(\boldsymbol{q}) u^{\dagger}(\boldsymbol{q}), \tag{11}$$

with

$$u(\boldsymbol{q}) = b_{\boldsymbol{q}} + b^{\dagger}_{-\boldsymbol{q}}. \tag{12}$$

Contrary to (9), the interaction considered in (11) does not preserve the number of quanta of the macroscopic system and rather than a collisional interaction describes, e.g., a Fröhlich-type interaction between electron and phonon [25].

2. Comparison with the Caldeira-Leggett model

Before showing the relationship between the above introduced translationally invariant interactions and corresponding structures of the master equation in the Markovian, weak-coupling limit, we briefly discuss the connection with the most famous Caldeira-Leggett model for the quantum description of dissipation and decoherence. Despite, or equivalently because of, its widespread use and relevance in applications, it is well worth trying to elucidate the basic physics behind the model, at least restricted to specific situations. In the standard formulation of the Caldeira-Leggett model (see for example [26–28]) the Hamiltonian for the environment is given in first quantization by the expression

$$H_{\rm M} = \sum_{i=1}^{N}\left(\frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2 x_i^2\right), \tag{13}$$

which should describe a set of independent harmonic oscillators, while the interaction term is given by (here and in the following we denote one-particle operators referring to the test particle with a caret)

$$V_{\rm PM} = -\hat{\mathsf{x}}\sum_{i=1}^{N} c_i x_i + \hat{\mathsf{x}}^2\sum_{i=1}^{N}\frac{c_i^2}{2m_i\omega_i^2}, \tag{14}$$

typically focusing on a one-dimensional system, where the first term is a position-position coupling and the second one is justified as a counterterm necessary in order to restore the physical frequencies of the dynamics of the microsystem, given for example by a Brownian particle. In the absence of an external potential for the test particle it is also observed that translational invariance, explicitly broken by Eqs. (13) and (14), can be recovered by suitably fixing the otherwise arbitrary coupling constants c_i to be given by $c_i = m_i\omega_i^2$ [27], which should not affect the relevant results which actually depend only on the so-called spectral density

$$J(\omega) = \sum_{i=1}^{N}\frac{c_i^2}{2m_i\omega_i}\delta(\omega - \omega_i), \tag{15}$$

which as a matter of fact is phenomenologically fixed. Since the original idea behind the model is to give an effective description of quantum dissipation in which the phenomenological quantities are to be fixed by comparison with the classical model, thus working in a semiclassical spirit, recovery of quantum Brownian motion in the sense of Einstein in the case of a test particle in a homogeneous medium is a natural requirement, and in fact the master equation obtained from the Caldeira-Leggett model with the Ohmic prescription for Eq. (15) is considered as the standard quantum description of Brownian motion. Nonetheless, as stressed in [14], despite the aforementioned *ad hoc* adjustments the Caldeira-Leggett model does not comply with one of the basic features of Brownian motion, i.e., translational invariance, and in fact also previous work has focused on how to recover translational invariance in the quantum description of dissipation [29]. In their analysis the authors of [14] try to recover a modified, translationally invariant version of the Caldeira-Leggett model by exploiting a suitable limit of an interaction of the density-displacement type considered above in Eq. (11). While this model might be the correct one for other physical systems, we claim that Einstein's quantum Brownian motion corresponds to a density-density coupling and we now see how the Caldeira-Leggett model is related to the long-wavelength limit of a density-density coupling.

Let us in fact consider Eq. (9), restricting the expressions to the one-particle sector for the test particle and to the N-particle sector for the macroscopic system, thus obtaining, using a first quantization formalism as in the Caldeira-Leggett model,

$$V_{\rm PM} = \sum_{i=1}^{N} t(\hat{\mathsf{x}} - \boldsymbol{x}_i) = \int d^3\boldsymbol{q}\,\tilde{t}(\boldsymbol{q})\sum_{i=1}^{N} e^{-(i/\hbar)\boldsymbol{q}\cdot(\hat{\mathsf{x}} - \boldsymbol{x}_i)}. \tag{16}$$

Considering only small momentum transfers and thus taking the long-wavelength limit of the expression, corresponding to a collective response of the macroscopic medium, one obtains up to second order

$$V_{\rm PM} \overset{\rm LWL}{\approx} N\int d^3\boldsymbol{q}\,\tilde{t}(\boldsymbol{q}) - \frac{1}{2\hbar^2}\int d^3\boldsymbol{q}\,\tilde{t}(\boldsymbol{q})\sum_{i=1}^{N}[\boldsymbol{q}\cdot(\hat{\mathsf{x}} - \boldsymbol{x}_i)]^2 + O(q^4), \tag{17}$$

where the term linear in $\boldsymbol{q}$ has dropped out because of inversion symmetry. Further exploiting isotropy, so that $\tilde{t}(\boldsymbol{q}) = \tilde{t}(q)$, one has

$$V_{\mathrm{PM}} \overset{\mathrm{LWL}}{\approx} Nt(0) - \frac{1}{3}\Delta_2 t(0)\hat{\mathsf{x}} \cdot \sum_{i=1}^{N} \boldsymbol{x}_i + \frac{1}{6}\Delta_2 t(0) \sum_{i=1}^{N} \boldsymbol{x}_i^2 + \frac{N}{6}\Delta_2 t(0)\hat{\mathsf{x}}^2 + O(q^4). \tag{18}$$

Here one easily recognizes the Caldeira-Leggett model, though with some constraints and modifications. First of all, as evident from Eq. (16) and also stressed in [14], translational invariance is preserved in the long-wavelength limit only provided that all terms up to a given order in $\boldsymbol{q}$ are consistently kept, and this also applies to any calculation put forward by means of Eq. (18). This explains the appearance of the so-called counterterm in Eq. (14), as well as the relationship $c_i = m_i \omega_i^2$ required in order to apparently restore translational invariance. The symmetry requirement thus strictly fixes the relationship between coefficients. However, a position-position coupling such as the one appearing in Eq. (18) is the common feature of the long-wavelength limit of a density-density coupling with a generic, not necessarily harmonic, potential. In the case in which the potential is harmonic, $t(\boldsymbol{x}) = \frac{1}{2} m\omega^2 \boldsymbol{x}^2$, one obtains from Eq. (18)

$$V_{\mathrm{PM}} \overset{\mathrm{LWL}}{\approx} \frac{1}{2} m\omega^2 \sum_{i=1}^{N} (\boldsymbol{x}_i^2 + \hat{\mathsf{x}}^2) - m\omega^2 \hat{\mathsf{x}} \cdot \sum_{i=1}^{N} \boldsymbol{x}_i \tag{19}$$

as in [27]. Let us note how in Eq. (18) the test particle couples to the collective coordinate

$$\boldsymbol{X} = \sum_{i=1}^{N} \boldsymbol{x}_i \tag{20}$$

of the macroscopic system, proportional to its center of mass. In a truly quantum picture of Einstein's Brownian motion, the gas has to be described by identical particles (or mixtures thereof), so that one cannot introduce different masses and different coupling constants. According to Eq. (9) or (16) in a density-density interaction the test particle is differently coupled to the various $\boldsymbol{q}$ components of the number-density operator for the macroscopic system $\rho_{\boldsymbol{q}}$, depending on the specific expression of the interaction potential $t(\boldsymbol{x})$. Of course this is no longer relevant when interpreting the harmonic oscillators as representatives of possible modes of the macroscopic system. Here and in the following we are not aiming at a general critique of the Caldeira-Leggett model, which obviously has big merits, let alone its historical meaning as a pioneering work in research on quantum dissipation. Rather, focusing on the particular and at the same time paradigmatic example of the quantum description of Einstein's Brownian motion, we want to put into evidence the possible detailed microscopic physics behind the model, especially in view of natural symmetry requirements, thus also opening the way for alternative ways to look at and cope with dissipation and decoherence in quantum mechanics, especially overcoming the limitation to Gaussian statistics inherent in the Caldeira-Leggett model. The relevance that the microphysical coupling actually has in determining which physical phenomena can be correctly described by a given model has also been stressed in [15], where an analysis is made of pure decoherence without dissipation, indicating that a full density-density coupling rather than a position-position coupling as in the Caldeira-Leggett model (in the paper correctly formalized in terms of a Bose field) should provide the proper way to describe pure, recoiless decoherence.

B. Structure of translation-covariant quantum-dynamical semigroups

We now come back to the translationally invariant interactions given by Eqs. (9) and (11), showing the possible master equations they lead to in the Markovian, weak-coupling limit. To do this we first observe that because of homogeneity of the underlying medium and translational invariance of the interaction potential, the reduced dynamics of the test particle must also be invariant under translations. This symmetry requirement has to be reflected in the actual structure of the master equation, i.e., the generator of the irreversible dynamics. The natural way to comply with this symmetry requirement is to ask the generator of the quantum-dynamical semigroup driving the dynamics of the test particle to be covariant under translations, i.e., that its action on the statistical operator commutes with the action of the unitary representation of translations. A more precise statement of covariance can be given as follows. Given the unitary representation $\hat{\mathsf{U}}(\boldsymbol{a}) = \exp[-(i/\hbar)\boldsymbol{a}\cdot\hat{\mathsf{p}}]$, $\mathbf{a} \in \mathbb{R}^3$, of the group of translations $\mathbb{R}^3$ in the test particle Hilbert space, a mapping $\mathcal{L}$ acting on the statistical operators in this space is said to be translation covariant if it commutes with the action of the unitary representation, i.e.,

$$\mathcal{L}[\hat{\mathsf{U}}(\boldsymbol{a})\hat{\varrho}\hat{\mathsf{U}}^\dagger(\boldsymbol{a})] = \hat{\mathsf{U}}(\boldsymbol{a})\mathcal{L}[\hat{\varrho}]\hat{\mathsf{U}}^\dagger(\boldsymbol{a}), \tag{21}$$

for any statistical operator $\hat{\varrho}$ and any translation $\boldsymbol{a}$. Needless to say, the notion of covariance under a given symmetry group has proved very powerful in characterizing not only mappings such as quantum-dynamical semigroups and operations, but also observables, especially in the generalized sense of positive-operator-valued measures [30,31]. As has been shown in recent, seminal work by Holevo [10,32–34], it turns out that the requirement of translation covariance puts very stringent constraints on the general possible structure of generators of quantum-dynamical semigroups. These results, while obviously fitting in the general framework set by the famous Lindblad result [35,36], go beyond it, giving much more detailed information on the possible choice of operators appearing in the Lindblad form, information conveyed by the symmetry requirements and relying on a quantum generalization of the Lévy-Khintchine formula. They therefore also provide a valuable starting point for phenomenological approaches exploiting relevant physical symmetries.

Referring to the papers by Holevo for the related mathematical details (see also [37] for a brief resume), the main structure of the generator can be expressed as

$$\mathcal{L}[\hat{\varrho}] = -\frac{i}{\hbar}[H(\hat{\mathsf{p}}), \hat{\varrho}] + \mathcal{L}_G[\hat{\varrho}] + \mathcal{L}_P[\hat{\varrho}], \tag{22}$$

with $H(\hat{\mathsf{p}})$ a self-adjoint operator which is a function of only the momentum of the test particle. The so-called Gaussian part $\mathcal{L}_G$ is given by

$$\mathcal{L}_G[\hat{\varrho}] = -\frac{i}{\hbar}[\hat{\mathsf{y}}_0 + H_{\mathrm{eff}}(\hat{\mathsf{x}},\hat{\mathsf{p}}),\hat{\varrho}] + \sum_{k=1}^{r}\left[K_k\hat{\varrho}K_k^\dagger - \frac{1}{2}\{K_k^\dagger K_k,\hat{\varrho}\}\right], \tag{23}$$

where

$$K_k = \hat{\mathsf{y}}_k + L_k(\hat{\mathsf{p}}),$$

$$\hat{\mathsf{y}}_k = \sum_{i=1}^{3} a_{ki}\hat{\mathsf{x}}_i, \quad k = 0,\ldots,r \leqslant 3, \quad a_{ki} \in \mathbb{R},$$

$$H_{\mathrm{eff}}(\hat{\mathsf{x}},\hat{\mathsf{p}}) = \frac{\hbar}{2i}\sum_{k=1}^{r}[\hat{\mathsf{y}}_k L_k(\hat{\mathsf{p}}) - L_k^\dagger(\hat{\mathsf{p}})\hat{\mathsf{y}}_k],$$

while the remaining Poisson part takes the form

$$\mathcal{L}_P[\hat{\varrho}] = \int d\mu(\boldsymbol{q})\sum_{j=1}^{\infty}\left[e^{(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}}L_j(\boldsymbol{q},\hat{\mathsf{p}})\hat{\varrho}L_j^\dagger(\boldsymbol{q},\hat{\mathsf{p}})e^{-(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}} - \frac{1}{2}\{L_j^\dagger(\boldsymbol{q},\hat{\mathsf{p}})L_j(\boldsymbol{q},\hat{\mathsf{p}}),\hat{\varrho}\}\right], \tag{24}$$

with $d\mu(\boldsymbol{q})$ a positive measure, and $\hat{\mathsf{x}}$ and $\hat{\mathsf{p}}$ position and momentum operators for the test particle respectively. The names Gaussian and Poisson arise in connection with the different parts related to the homonymous stochastic processes in the classical Lévy-Khintchine formula. In the Gaussian part the $\hat{\mathsf{y}}_k$ are linear combinations of the position operators of the test particle, which thus appear at most linearly in the commutator term, and bilinearly in the rest of the expression. The generally complex functions $L_k(\hat{\mathbf{p}})$ have an imaginary part describing friction, typically given by a linear contribution, corresponding to a friction term proportional to velocity. In the Poisson part a continuous index $\boldsymbol{q}$ appears, together with the usual sum over a discrete index j. The expression is characterized by the appearance of the unitary operators $\exp[(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}]$, acting as generators of boosts or momentum translations, and of the functions $L_j(\boldsymbol{q},\hat{\mathsf{p}})$, operator valued in that they depend on the momentum operators of the test particle $\hat{\mathbf{p}}$, i.e., the generators of translations.

As can be seen the characterization is quite powerful, so that the only freedom left is in the choice of a few coefficients and functions of the momentum operators of the test particle $\hat{\mathsf{p}}$. These can be fixed by either referring to microphysical calculations, or relying on a suitably guessed phenomenological ansatz. In this kind of reduced dynamics the information on the macroscopic system the test particle is interacting with is essentially encoded in a suitable, possibly operator-valued, two-point correlation function of the macroscopic system appearing in the Lindblad structure. The key physical point is then the identification of the relevant two-point correlation function, depending both on the coupling between test particle and reservoir, and on a characterization of the equilibrium state of the reservoir.

C. Physical examples

Building on the results of Secs. II A and II B we will now give two examples of physical realization of the previously outlined structures, corresponding to the couplings (9) and (11). In this way we show how apparently very different results obtained in the literature can be put in a unified framework, putting into evidence the common root due to translational invariance and thus suggesting how to handle similar situations characterized by the same symmetry group.

The case of density-density coupling given by Eq. (9), when the reservoir is a free quantum gas, has been dealt with in [11–13], and the relevant test particle correlation function turns out to be the so-called dynamic structure factor [21,22]

$$S(\boldsymbol{q},E) = \frac{1}{2\pi\hbar}\frac{1}{N}\int dt e^{(i/\hbar)Et}\langle\rho_{\boldsymbol{q}}^\dagger\rho_{\boldsymbol{q}}(t)\rangle, \tag{25}$$

which can be written in an equivalent way as

$$S(\boldsymbol{q},E) = \frac{1}{N}\sum_{mn}\frac{e^{-\beta E_n}}{\mathcal{Z}}|\langle m|\rho_q|n\rangle|^2\delta(E + E_m - E_n), \tag{26}$$

where contrary to the usual conventions, momentum and energy are considered to be positive when transferred to the test particle, on which we are now focusing our attention, rather than on the macroscopic system. The master equation then takes the form

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar}[\hat{\mathsf{H}}_0,\hat{\varrho}] + \frac{2\pi}{\hbar}(2\pi\hbar)^3 n\int d^3\boldsymbol{q}|\tilde{t}(q)|^2 \times\left[e^{(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}}\sqrt{S(\boldsymbol{q},E(\boldsymbol{q},\hat{\mathsf{p}}))}\hat{\varrho}\sqrt{S(\boldsymbol{q},E(\boldsymbol{q},\hat{\mathsf{p}}))} \times e^{-(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}} - \frac{1}{2}\{S(\boldsymbol{q},E(\boldsymbol{q},\hat{\mathsf{p}})),\hat{\varrho}\}\right], \tag{27}$$

where $\hat{\mathsf{H}}_0$ is the free particle Hamiltonian, n is the density of the homogeneous gas, and the dynamic structure factor appears operator valued: in fact the energy transfer in each collision, which is given by

$$E(\boldsymbol{q},\boldsymbol{p}) = \frac{(\boldsymbol{p}+\boldsymbol{q})^2}{2M} - \frac{\boldsymbol{p}^2}{2M}, \tag{28}$$

with M the mass of the test particle, is turned into an operator by replacing $\boldsymbol{p}$ with $\hat{\mathsf{p}}$. For the case of a free gas of particles obeying Maxwell-Boltzmann statistics the dynamic structure factor takes the explicit form

$$S_{\mathrm{MB}}(\boldsymbol{q},E) = \sqrt{\frac{\beta m}{2\pi}}\frac{1}{q}e^{-(\beta/8m)(2mE + q^2)^2/q^2} \tag{29}$$

with β the inverse temperature and m the mass of the gas particles.

A density-displacement type of coupling as in Eq. (11) has been dealt with in [38,39], considering an environment essentially given by a phonon bath. The relevant test particle correlation function in this kind of model is given by the following spectral function [21,24]:

$$S(\boldsymbol{q},E) = \frac{1}{2\pi\hbar}\int dt\, e^{(i/\hbar)Et}\langle u^\dagger(\boldsymbol{q})u(\boldsymbol{q},t)\rangle, \tag{30}$$

given by a linear combination of correlation functions of the form

$$A(\boldsymbol{q},E) = \frac{1}{2\pi\hbar}\int dt\, e^{(i/\hbar)Et}\langle b_{\boldsymbol{q}}^{\dagger} b_{\boldsymbol{q}}(t)\rangle, \tag{31}$$

which can also be written [40]

$$A(\boldsymbol{q},E) = \sum_{mn} \frac{e^{-\beta E_n}}{\mathcal{Z}} |\langle m|b_{\boldsymbol{q}}|n\rangle|^2 \delta(E + E_m - E_n). \tag{32}$$

Contrary to the smooth expression of the dynamic structure factor for a free quantum gas given in Eq. (29), the spectral function (31) has the highly singular structure

$$S(\boldsymbol{q},E) = [1 + N_\beta(\hbar\omega_{\boldsymbol{q}})]\delta(E + \hbar\omega_{\boldsymbol{q}}) + N_\beta(\hbar\omega_{\boldsymbol{q}})\delta(E - \hbar\omega_{\boldsymbol{q}}), \tag{33}$$

with $N_\beta(\hbar\omega_{\boldsymbol{q}}) = 1/(e^{\beta\hbar\omega_{\boldsymbol{q}}} - 1)$, where the exact frequencies $\hbar\omega_{\boldsymbol{q}}$ of the phonon appear. The smooth energy dependence of the test particle correlation function used in the derivation of Eq. (27), allowing an exact treatment in the case of a free gas of Maxwell-Boltzmann particles, here no longer applies, and in fact the master equation has only been worked out for the diagonal matrix elements of the statistical operator in the momentum representation. Setting $\varrho(\boldsymbol{p}) \equiv \langle \boldsymbol{p}|\hat{\varrho}|\boldsymbol{p}\rangle$ one has

$$\frac{d\varrho}{dt}(\boldsymbol{p}) = \int d^3\boldsymbol{q} |\tilde{t}(q)|^2 [S(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}-\boldsymbol{q}))\varrho(\boldsymbol{p}-\boldsymbol{q}) - S(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))\varrho(\boldsymbol{p})], \tag{34}$$

using the notation introduced in Eq. (28). One immediately sees that both (27) and (34) fit in the general expression (24) for the Poisson part of the generator of a translation-covariant quantum-dynamical semigroup given by Holevo, with the $|L_j(\boldsymbol{q},\hat{\mathsf{p}})|^2$ operators replaced by the spectral functions (25) and (30), respectively, the integration measure $d\mu(\boldsymbol{q})$ corresponding to the Lebesgue measure with a weight given by the square modulus of the Fourier transform of the interaction potential. It is here already apparent that the presented results (27) and (34), pertaining to the Poisson part (24) of the general structure of the generator of a translation-covariant quantum-dynamical semigroup (22), go beyond the limitation to Gaussian statistics typical of the Caldeira-Leggett model.

The relevant correlation function for these translation-covariant master equations thus appears to be given by the Fourier transform with respect to energy of the time-dependent autocorrelation function of the operator of the macroscopic system appearing in the interaction potential V_{PM} when written in the form (5), i.e.,

$$S(\boldsymbol{q},E) = \frac{1}{2\pi\hbar}\int dt\, e^{(i/\hbar)Et}\langle A_{\mathrm{M}}^{\dagger}(\boldsymbol{q})A_{\mathrm{M}}(\boldsymbol{q},t)\rangle. \tag{35}$$

The parameter $\boldsymbol{q}$ one integrates over in Eq. (24), with a weight given by the square modulus of the Fourier transform of the interaction potential appearing in Eq. (5), is to be seen as an element of the translation group, physically corresponding to the possible momentum transfers in the single collisions. The key difference between the two models lies in the physical meaning of the different correlation functions. The dynamic structure factor (25) is linked to the so-called density fluctuations spectrum, accounting for particle number conservation of the macroscopic system. This connection to density fluctuations brings into play the other key feature of Einstein's Brownian motion, i.e., the molecular, discrete nature of matter. As we shall see shortly, the smooth correlation function arising in connection with this density-density coupling allows us to take a diffusive limit of the reduced dynamics, thus obtaining the quantum description of Einstein's Brownian motion. On the contrary in Eq. (30) the typically quantized spectrum of a harmonic oscillator appears, thus leading to the singular function (33), so that as stressed in [39] rather than a diffusion equation one necessarily has a jump process.

III. FLUCTUATION-DISSIPATION THEOREM

In the previous section we have tried to point out and analyze the typical structures for the quantum description of dissipation and decoherence in the Markovian case that come into play when the first of the two key features of Einstein's Brownian motion mentioned in Sec. I is taken into account, i.e., translational invariance. We now focus on the second key feature, i.e., the connection with the discrete nature of matter, which Einstein actually wanted to demonstrate. As already hinted at the end of Sec. (2), in the present paper we substantiate the claim that the correct description of Einstein's Brownian motion is obtained considering a density-density coupling. As we shall see in detail in Sec. IV this happens thanks to the fact that the two-point correlation function appearing in the master equation in this case is the dynamic structure factor (25), where the Fourier transform of the number-density operator $\rho_{\boldsymbol{q}}$, as given in Eq. (8), appears. This function is in fact directly related to the density fluctuations in the medium, as can be seen in writing it, rather than in the form (25), relevant for the comparison between the different types of translational invariance interactions and related master equations, in the following way [21]:

$$S(\boldsymbol{q},E) = \frac{1}{2\pi\hbar}\int dt \int d^3\boldsymbol{x}\, e^{i/\hbar(Et - \boldsymbol{q}\cdot\boldsymbol{x})} G(\boldsymbol{x},t), \tag{36}$$

i.e., as the Fourier transform with respect to energy and momentum transfer of the time-dependent density correlation function

$$G(\boldsymbol{x},t) = \frac{1}{N}\int d^3\boldsymbol{y}\langle N_{\mathrm{M}}(\boldsymbol{y})N_{\mathrm{M}}(\boldsymbol{x}+\boldsymbol{y},t)\rangle. \tag{37}$$

Here the connection with density fluctuations and therefore the discrete nature of matter is manifest. Introducing the real correlation functions

$$\phi^{-}(\boldsymbol{q},t) = \frac{i}{\hbar N}\langle[\rho_{\boldsymbol{q}}(t),\rho_{\boldsymbol{q}}^{\dagger}]\rangle,$$

$$\phi^{+}(\boldsymbol{q},t) = \frac{1}{\hbar N}\langle\{\rho_{\boldsymbol{q}}(t),\rho_{\boldsymbol{q}}^{\dagger}\}\rangle, \tag{38}$$

where $\{\ ,\ \}$ denotes the anticommutator, the fluctuation-dissipation theorem can be formulated in terms of the dynamic structure factor as follows:

$$\phi^{-}(\boldsymbol{q},t) = -\frac{2}{\hbar}\int_{-\infty}^{0} dE \sin\left(\frac{E}{\hbar}t\right)(1-e^{\beta E})S(\boldsymbol{q},E),$$

$$\phi^{+}(\boldsymbol{q},t) = -\frac{2}{\hbar}\int_{-\infty}^{0} dE \cos\left(\frac{E}{\hbar}t\right)\coth\left(\frac{\beta}{2}E\right)(1-e^{\beta E})S(\boldsymbol{q},E). \tag{39}$$

We stress once again that contrary to the usual perspective in linear response theory, we are here concerned with the reduced dynamics of the test particle, so that we take as positive the momentum and energy transferred to the particle. The dynamic structure factor can also be directly related to the dynamic response function $\chi''(\boldsymbol{q},E)$ [22], according to

$$S(\boldsymbol{q},E) = \frac{1}{2\pi}\left[1-\coth\left(\frac{\beta}{2}E\right)\right]\chi''(\boldsymbol{q},E) = \frac{1}{\pi}\frac{1}{1-e^{\beta E}}\chi''(\boldsymbol{q},E), \tag{40}$$

the relationship leading to the important fact that while the dynamic response function is an odd function of energy, the dynamic structure factor obeys the so-called detailed balance condition

$$S(\boldsymbol{q},E) = e^{-\beta E}S(-\boldsymbol{q},-E), \tag{41}$$

a property granting the existence of a stationary state for the master equation (27), as shown in [13]. In terms of the dynamic response function the fluctuation-dissipation theorem can also be written

$$\phi^{-}(\boldsymbol{q},t) = -\frac{2}{\pi\hbar}\int_{-\infty}^{0} dE \sin\left(\frac{E}{\hbar}t\right)\chi''(\boldsymbol{q},E),$$

$$\phi^{+}(\boldsymbol{q},t) = -\frac{2\pi}{\hbar}\int_{-\infty}^{0} dE \cos\left(\frac{E}{\hbar}t\right)\coth\left(\frac{\beta}{2}E\right)\chi''(\boldsymbol{q},E), \tag{42}$$

a formulation that will prove useful for later comparison with the Caldeira-Leggett model. The most significant formulation of the so-called fluctuation-dissipation theorem for the physics we are considering is, however, neither (39) nor (42), but is to be traced back to a seminal paper by Van Hove [9,24]. In fact he showed that the scattering cross section of a microscopic probe off a macroscopic sample can be written in Born approximation in the following way:

$$\frac{d^2\sigma}{d\Omega_{p'}dE_{p'}}(\boldsymbol{p}) = (2\pi\hbar)^6\left(\frac{M}{2\pi\hbar^2}\right)^2\frac{p'}{p}|\tilde{t}(q)|^2 S(\boldsymbol{q},E), \tag{43}$$

where a particle of mass M changes its momentum from $\boldsymbol{p}$ to $\boldsymbol{p}'=\boldsymbol{p}+\boldsymbol{q}$ scattering off a medium with dynamic structure factor $S(\boldsymbol{q},E)$. This is the most pregnant formulation of the fluctuation-dissipation relationship for the case of a test particle interacting through collisions with a macroscopic fluid. The energy and momentum transfer to the particle, characterized by the expression of the scattering cross section on the left-hand side (LHS) of Eq. (43) are related to the density fluctuations of the macroscopic fluid appearing through the dynamic structure factor on the RHS of Eq. (43). One of the basic ideas of Einstein's Brownian motion, i.e., the discrete nature of matter, once again appears in the formulation (43) of the fluctuation-dissipation relationship. From the comparison between Eqs. (43) and (27) one sees that the reduced dynamics is actually driven by the collisional scattering cross section; in particular the last term of Eq. (27) can also be written

$$-\frac{n}{2M}\{|\hat{\mathsf{p}}|\sigma(\hat{\mathsf{p}}),\hat{\varrho}\}, \tag{44}$$

where $\sigma(\boldsymbol{p})$ is the total macroscopic scattering cross section obtained from the differential expression (43) for a test particle with incoming momentum $\boldsymbol{p}$. The term (44) can be seen quite naturally as a loss term in a kinetic equation, and in fact Eq. (27) is actually to be seen as a quantum version of the linear Boltzmann equation [41]. Besides this, from the direct relation (43) between the scattering cross section and dynamic structure factor one sees on physical grounds the positivity of the correlation function, a property exploited in (27) in order to take the square root.

We now compare the above formulations of the fluctuation-dissipation theorem with the ones encountered in the long-wavelength limit of the density-density coupling type of translationally invariant interaction, which as shown in Sec. II A 2 is strongly related to the Caldeira-Leggett model. In the long-wavelength limit the $\boldsymbol{q}$ component of the number-density operator becomes

$$\rho_{\boldsymbol{q}} \overset{\text{LWL}}{\approx} N - \frac{i}{\hbar}\boldsymbol{q}\cdot\sum_{i=1}^{N}\boldsymbol{x}_i + O(q^2), \tag{45}$$

and once again the collective coordinate $\boldsymbol{X}=\sum_{i=1}^{N}\boldsymbol{x}_i$ introduced in Eq. (20) is put into evidence. The relevant correlation functions then become

$$\phi_{ij}^{-}(t) = \frac{i}{\hbar N}\langle[\boldsymbol{X}_i(t),\boldsymbol{X}_j]\rangle,$$

$$\phi_{ij}^{+}(t) = \frac{1}{\hbar N}\langle\{\boldsymbol{X}_i(t),\boldsymbol{X}_j\}\rangle, \tag{46}$$

the indexes i and j here denoting Cartesian components of the collective coordinate (20). Introducing accordingly the spectral function

$$S_{ij}(E) = \frac{1}{2\pi\hbar}\frac{1}{N}\int dt\, e^{(i/\hbar)Et}\langle\boldsymbol{X}_j\boldsymbol{X}_i(t)\rangle, \tag{47}$$

the fluctuation-dissipation theorem reads

$$\phi_{ij}^{-}(t) = -\frac{2}{\hbar}\int_{-\infty}^{0} dE \sin\left(\frac{E}{\hbar}t\right)(1-e^{\beta E})S_{ij}(E),$$

$$\phi_{ij}^{+}(t) = -\frac{2}{\hbar}\int_{-\infty}^{0} dE \cos\left(\frac{E}{\hbar}t\right)\coth\left(\frac{\beta}{2}E\right)(1-e^{\beta E})S_{ij}(E). \tag{48}$$

With the help of the response function $\chi_{ij}''(E)$

$$S_{ij}(E) = \frac{1}{\pi}\frac{1}{1-e^{\beta E}}\chi''_{ij}(E), \qquad (49)$$

the relations (48) can also be written as

$$\phi^-_{ij}(t) = -\frac{2}{\pi\hbar}\int_{-\infty}^{0} dE \sin\left(\frac{E}{\hbar}t\right)\chi''_{ij}(E),$$

$$\phi^+_{ij}(t) = -\frac{2}{\pi\hbar}\int_{-\infty}^{0} dE \cos\left(\frac{E}{\hbar}t\right)\coth\left(\frac{\beta}{2}E\right)\chi''_{ij}(E). \qquad (50)$$

While a formulation of the fluctuation-dissipation theorem like the Van Hove relation (43) is missing in this long-wavelength limit, the relations (50), involving expectation values of the commutator and anticommutator of the components of the collective coordinates, are the ones to be compared with the typical relations used in order to introduce the so-called spectral density (15) in the Caldeira-Leggett model. In fact if all coupling constants c_i are put equal to c, as should be enforced in the case of Einstein's quantum Brownian motion, in which the particle interacts through collisions with a collection of identical, indistinguishable particles, the spectral density, when expressed in terms of energy E rather than frequency ω, will be related to the response function $\chi''(E)$ for a one-dimensional system according to

$$J(E) = \frac{c^2}{\pi}\chi''(E). \qquad (51)$$

The relation (51), first intuitively guessed in [42], actually shows how in the friction coefficient, usually phenomenologically introduced through the spectral density, features of both the single interaction events and the reservoir do appear. In Sec. IV we will give a microscopic expression for the friction coefficient in the case of Einstein's quantum Brownian motion, in which both features do appear: the coupling through the Fourier components of the interaction potential, and the reservoir through certain values of the dynamic structure factor.

IV. QUANTUM DESCRIPTION OF EINSTEIN'S BROWNIAN MOTION

Relying on the premises of Secs. II and III we now come to the master equation for the quantum description of Einstein's Brownian motion. The requirement of translational invariance has been settled in Sec. II, while the connection between the reduced dynamics of the test particle and density fluctuations in the medium, coming about because of its discrete nature, has been taken into account in Sec. III, considering a density-density coupling and thus coming to Eq. (27). The last step to be taken is to consider the test particle much more massive than the particles making up the gas, i.e., the Brownian limit $m/M \ll 1$, which in turn implies considering energy and momentum transfers that are both small, similarly to the classical case [43]. We therefore start from Eq. (27) and consider a free gas of Maxwell-Boltzmann particles, so that taking the limiting expression of (29) when the ratio between the masses is much smaller than 1, or equivalently considering small energy transfers, i.e.,

$$S^{\infty}_{\rm MB}(\boldsymbol{q},E) = \sqrt{\frac{\beta m}{2\pi}}\frac{1}{q}e^{-(\beta/8m)q^2}e^{-(\beta/2)E}, \qquad (52)$$

one obtains the master equation [11–13]

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar}[\hat{\mathsf{H}}_0,\hat{\varrho}] + \frac{2\pi}{\hbar}(2\pi\hbar)^3 n\sqrt{\frac{\beta m}{2\pi}}\int d^3\boldsymbol{q}\frac{|\tilde{t}(q)|^2}{q} \times e^{-(\beta/8m)(1+2m/M)q^2}\left[e^{(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}}e^{-(\beta/4M)\boldsymbol{q}\cdot\hat{\mathsf{p}}}\hat{\varrho}e^{-(\beta/4M)\boldsymbol{q}\cdot\hat{\mathsf{p}}} \times e^{-(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}} - \frac{1}{2}\left\{e^{-(\beta/2M)\boldsymbol{q}\cdot\hat{\mathsf{p}}},\hat{\varrho}\right\}\right], \qquad (53)$$

which in the limit of small momentum transfer leads, of necessity as can be seen from the Gaussian contribution in Holevo's result (23) but also from previous work [6,7], to a Caldeira-Leggett type of master equation, but without the shortcomings related to the lack of preservation of positivity of the statistical operator. The master equation takes the form

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar}[\hat{\mathsf{H}}_0,\hat{\varrho}] - \frac{i}{\hbar}\frac{\eta}{2}\sum_{i=1}^{3}[\hat{\mathsf{x}}_i,\{\hat{\mathsf{p}}_i,\hat{\varrho}\}] - \frac{D_{pp}}{\hbar^2}\sum_{i=1}^{3}[\hat{\mathsf{x}}_i,[\hat{\mathsf{x}}_i,\hat{\varrho}]] - \frac{D_{xx}}{\hbar^2}\sum_{i=1}^{3}[\hat{\mathsf{p}}_i,[\hat{\mathsf{p}}_i,\hat{\varrho}]], \qquad (54)$$

with

$$D_{pp} = \frac{M}{\beta}\eta \quad \text{and} \quad D_{xx} = \frac{\beta\hbar^2}{16M}\eta. \qquad (55)$$

The friction coefficient η is uniquely determined on the basis of the microscopic information on the interaction potential and correlation function of the macroscopic system, according to

$$\eta = \frac{\beta}{2M}\frac{2\pi}{\hbar}(2\pi\hbar)^3 n\int d^3\boldsymbol{q}|\tilde{t}(q)|^2\frac{q^2}{3}S(\boldsymbol{q},E=0), \qquad (56)$$

the factor 3 being related to the space dimensions, or equivalently

$$\eta = \frac{\beta}{2M}\frac{2\pi}{\hbar}(2\pi\hbar)^2 n\int d^3\boldsymbol{q}|\tilde{t}(q)|^2\frac{q^2}{3}\frac{1}{N}\int dt\langle\rho^\dagger_{\boldsymbol{q}}\rho_{\boldsymbol{q}}(t)\rangle, \qquad (57)$$

thus proving in a specific physical case of interest the so-called standard wisdom expecting the decoherence and dissipation rate to be connected with the value at zero energy of some suitable spectral function [15]. Introducing the Fourier transform of the gradient of the number-density operator, which we indicate by $\boldsymbol{\nabla}\rho_{\boldsymbol{q}}$

$$\boldsymbol{\nabla}\rho_{\boldsymbol{q}} \equiv \boldsymbol{q}\rho_{\boldsymbol{q}} = -i\hbar\int d^3\boldsymbol{x}\, e^{-(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{x}}\,\boldsymbol{\nabla}N_{\rm M}(\boldsymbol{x}), \qquad (58)$$

the friction coefficient can also be written in terms of the time-dependent autocorrelation function of $\nabla\rho_{\boldsymbol{q}}$ according to

$$\eta = \frac{\beta}{6M}\frac{2\pi}{\hbar}(2\pi\hbar)^2 n \int d^3\boldsymbol{q}|\tilde{t}(q)|^2 \frac{1}{N}\int dt \langle \nabla\rho_{\boldsymbol{q}}^\dagger \cdot \nabla\rho_{\boldsymbol{q}}(t)\rangle. \tag{59}$$

To the best of our knowledge these general expressions have been introduced here for the first time, providing a microphysical estimate of the friction coefficient η in terms of suitable correlation functions, through the two equivalent and both telling expressions (56) and (59).

It is worth noticing how, contrary to the usual Caldeira-Leggett model, the friction coefficient will generally exhibit an explicit temperature dependence, being related both to the expectation value of the operators $\rho_{\boldsymbol{q}}$ and to the interaction potential. No energy cutoff needs to be introduced, since all quantities appearing in the calculations remain finite, being directly linked to the relevant physical properties of the macroscopic system the test particle is interacting with. Note further that introducing the thermal momentum spread $\Delta p_{\mathrm{th}}^2 = M/\beta$ and the square thermal wavelength $\Delta x_{\mathrm{th}}^2 = \beta\hbar^2/4M$ satisfying the minimum uncertainty relation

$$\Delta p_{\mathrm{th}}\Delta x_{\mathrm{th}} = \frac{\hbar}{2}, \tag{60}$$

the coefficients given in Eq. (55) can also be expressed in the form

$$D_{pp} = \eta\Delta p_{\mathrm{th}}^2 \quad \text{and} \quad D_{xx} = \frac{\eta}{4}\Delta x_{\mathrm{th}}^2. \tag{61}$$

The main difference between Eq. (54) and the master equation introduced by Caldeira and Leggett for the description of quantum Brownian motion, apart from the microphysical expression for the appearing coefficients, lies in the appearance of the last contribution, given by a double commutator with the momentum operator of the Brownian particle, and corresponding to position diffusion. This term, which here appears in the expansion for small energy and momentum transfer of the dynamic structure factor, is directly linked to preservation of positivity of the statistical operator, and in fact in the past many different amendments of the Caldeira-Leggett master equation have been proposed in the literature introducing a term of this kind [11,44,45], even though it is not obvious how to actually experimentally check the relevance of this term, essentially quantum in origin, as can also be seen from Eqs. (60) and (61). In recent work [41] it has been shown how this contribution might lead in the strong friction limit to a typically quantum correction to Einstein's diffusion coefficient, only relevant at low temperatures, thus opening the way to the conception of future experiments in which to possibly check the correction, as considered in [46].

V. CONCLUSIONS AND OUTLOOK

In the present paper a fully quantum approach to the description of Brownian motion in the sense of Einstein, i.e., considering a massive test particle interacting through collisions with a background of much lighter ones, has been presented. The two cardinal requirements determining the quantum description of the reduced dynamics are translational invariance and the connection with the discrete, atomistic nature of the medium, along the lines of Einstein's original confrontation with the problem. The former implies the choice of a translationally invariant interaction potential and leads to the requirement of translation covariance for the quantum-dynamical semigroup giving the time evolution, a type of semigroup that has been fully characterized by Holevo [10] as seen in Sec. II; the latter relates the dynamics to the density fluctuations in the fluid, expressed in terms of the dynamic structure factor, first introduced by Van Hove [9], and ensuring the physically most telling formulation of the fluctuation-dissipation theorem for the considered case, as seen in Sec. III. A quantum master equation for the description of Einstein's Brownian motion, obtained in a kinetic approach complying with the abovementioned characteristics, has been given in Sec. IV, showing in particular how Einstein's quantum Brownian motion arises in the presence of a density-density coupling. This type of coupling fixes the relevant correlation function appearing in the microphysical expression obtained for the friction coefficient, given in Eq. (56) or equivalently Eq. (59).

A comparison has been drawn whenever possible between the present approach and the famous Caldeira-Leggett model for the treatment of decoherence and dissipation in quantum mechanics, showing how the Caldeira-Leggett model may arise as the long-wavelength limit of a density-density coupling preserving translational invariance. This accounts in particular for the limitation to Gaussian statistics inherent in the Caldeira-Leggett model or variants thereof. At variance with the Caldeira-Leggett model, a microphysical expression for the friction coefficient has been given, relating it to the Fourier transform of the interaction potential and a suitable autocorrelation function as seen in Sec. IV. No need of renormalizations or energy cutoffs appears in the treatment. Furthermore, physical realizations of the Poisson component of the general structure of generator of a translation-covariant quantum-dynamical semigroup (22) has been presented, going beyond the typical restriction to Gaussian statistics.

Even though focusing on the specific issue of Einstein's quantum Brownian motion, the results presented in Secs. II and III are quite general. They provide a clearcut connection between the expression of the translationally invariant interaction and precise structure of the associated reduced Markovian dynamics, satisfying the natural and physically compelling requirement of translation covariance. They further clarify the relevant correlation function of the environment for the reduced dynamics and its connection to the fluctuation-dissipation theorem, thus providing a general framework for a microphysical description of dissipation and decoherence in quantum mechanics. Now that experimental quantitative tests of decoherence begin to be within reach (see for example [16,47–49] or [26,50] for more general references), the next challenge for the theoretical analysis is in fact no longer an effective, phenomenological description of the phenomenon, but rather a full-fledged microphysical analysis, in which both the phenomena of dissipation and decoherence can be correctly described.

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