

# A quantum diffusion law

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We analyse diffusion at low temperature by bringing the fluctuation-dissipation theorem (FDT) to bear on a physically natural, viscous response-function  $R(t)$ . The resulting diffusion-law exhibits several distinct regimes of time and temperature, each with its own characteristic rate of spreading. As with earlier analyses, we find logarithmic spreading in the quantum regime, indicating that this behavior is robust. A consistent  $R(t)$  must satisfy the key physical requirements of *Wightman positivity* and *passivity*, and we prove that ours does so. We also prove in general that these two conditions are equivalent when the FDT holds. Given current technology, our diffusion law can be tested in a laboratory with ultra cold atoms.

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## I. INTRODUCTION

A Brownian particle suspended in a liquid subject to thermal fluctuations undergoes diffusion. What happens as we lower the temperature and scale down the size of the particle until we reach a regime where the diffusion is driven primarily by quantum zero point fluctuations?

The question of diffusion in the presence of quantum zero point fluctuations received a surge of interest in connection with gravitational wave detection [1]. Since such detectors need to work at high levels of precision, the analysis of the Brownian motion of the detector's components (such as mirrors) naturally comes into play [2–4].

In the present paper, we revisit this question starting — as before in our earlier paper [5] — from the fluctuation dissipation theorem. In contrast to Ref. [5], however, we consider here a response function whose behavior at very short times has been changed from a step function to one which is more consistent physically, and also closer to a form which is realizable in the laboratory. At the time when [5] was written, the predicted logarithmic diffusion was not experimentally accessible, but now that it is becoming so, it seems important to analyze a response function which is not only more realistic but also fully self-consistent.

The key physical requirements here are *Wightman positivity* of the position correlation function and *passivity*, which is essentially a version of the second law of thermodynamics. We define these conditions and discuss their interrelationships, showing in particular that they are equivalent when the fluctuation-dissipation theorem is in force. Unlike the response-function assumed in our earlier analysis, our present  $R(t)$  satisfies both Wightman positivity and passivity. This discussion, which is entirely new in relation to [5], demonstrates as well that  $R(t)$ , in addition to being natural from an experimental standpoint, is in principle realizable *exactly* as a quantum gaussian process.

In the last two decades, light-matter interaction has given a new impetus to such questions, and one can now cool dilute atomic gases down to temperatures of the or-

der of  $100nK$ , where the transition to quantum degenerate regime can be observed [6–11]. As we point out below, recent advances in experimental technique have progressed to the point that quantal diffusion effects should now be observable.

The paper is organized as follows. In Sec II we obtain analytically, the mean square displacement that results from our newer response function, relegating most of the computational details to the Appendix. In Sec III we describe certain positivity conditions that consistent correlation functions and response functions must satisfy, and we relate them to each other, showing that our more realistic response function does satisfy them. In Sec IV we review our main findings and discuss experimental possibilities.

## II. DIFFUSION LAW FROM FLUCTUATION DISSIPATION THEOREM: QUANTUM DIFFUSION FOR A REALISTIC RESPONSE FUNCTION

Our starting point is the fluctuation dissipation theorem (FDT), which in the frequency domain can be stated as follows [5, 12]:

$$\text{Im}\tilde{R}(\nu) = \frac{1}{\hbar} \tanh(\pi\beta\hbar\nu)\tilde{C}(\nu) \quad (1)$$

where,  $\beta = \frac{1}{k_B T}$  and  $\tilde{(\cdot)}$  denotes the *conjugate-linear* Fourier transform defined by

$$\tilde{f}(\nu) = \int dt e^{2\pi i\nu t} f^*(t).$$

$\tilde{R}(\nu)$  and  $\tilde{C}(\nu)$  are respectively the transforms of the time-dependent response-function  $R(t)$  and of the auto-correlation function  $C(t)$ :

$$R(t) = \frac{1}{i\hbar} \langle [x(0), x(t)] \rangle \theta(t) \quad (2)$$

$$C(t) = \frac{1}{2} \langle \{x(0), x(t)\} \rangle \quad (3)$$

where,  $x(t)$  is the displacement and  $\theta(t)$  is the unit step function defined as:

$$\theta(t) = \begin{cases} 1, & t \geq 0 \\ 0, & t < 0 \end{cases}$$

We now consider the fluctuation dissipation theorem in the time domain. To that end, we first consider, instead of  $R(t)$ , the equivalent odd function [5],

$$\check{R}(t) = \text{sgn}(t)R(|t|)$$

where  $\text{sgn}(t)$  is the sign or signum function, defined as:

$$\text{sgn}(t) = \begin{cases} 1, & t > 0 \\ 0, & t = 0 \\ -1, & t < 0 \end{cases}$$

$R(t)$  defined in Eq. (2) is a causal function which vanishes for  $t < 0$ , whereas  $\check{R}(t)$  exists for the entire time domain. This enables us to recast the fluctuation dissipation theorem as follows [5]:

$$\check{R}(\nu) = \frac{2i}{\hbar} \tanh(\pi\beta\hbar\nu)\check{C}(\nu) \quad (4)$$

We finally arrive at [5],

$$C(t) = \frac{1}{2\beta} \int_{-\infty}^{\infty} dt' \text{sgn}(t' - t)R(|t' - t|) \coth\left(\frac{\pi t'}{\beta\hbar}\right) + c \quad (5)$$

where  $c$  is a constant.

Our analysis focuses on the mean square displacement, and deduces it from the position auto-correlation function. The mean square displacement is given by,

$$\langle \Delta x^2 \rangle = \langle [x(t) - x(0)]^2 \rangle = 2[C(0) - C(t)] \quad (6)$$

Using Eq. (5), we can write [5],

$$\langle \Delta x^2 \rangle = \frac{1}{\beta} \int_0^{\infty} dt' R(t') \left\{ 2 \coth\left(\frac{t'}{t_{th}}\right) - \coth\left(\frac{t' + t}{t_{th}}\right) - \coth\left(\frac{t' - t}{t_{th}}\right) \right\} \quad (7)$$

where,  $t_{th} = \beta\hbar/\pi$  is the thermal time. The definition of mean square displacement in Eq. (6) entails that it is necessarily positive. This condition further restricts the choice of the response function, as we discuss more fully below.

We will consider primarily the following response-function:

$$R(t) = \mu \left(1 - e^{-\frac{t}{\tau}}\right) \theta(t) \quad (8)$$

Here  $\mu$  can be called the mobility and  $\tau$  the relaxation time. This response-function is suggested by the venerable model of a viscous medium. (Such a medium can be realized experimentally as a three-dimensional ‘‘optical molasses’’ of the type used for laser cooling of dilute

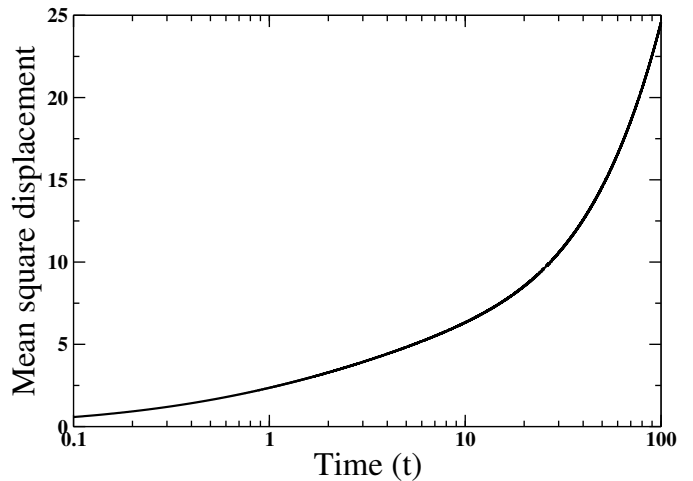


FIG. 1: Plot of the mean square displacement as a function of time (in logarithmic scale) in arbitrary units, obtained from Eq. (9). In this case, the relaxation time is taken to be  $\tau = 1$  and the thermal time is taken to be  $t_{th} = 10$ .

atomic gases [7].) Although (8) is not as easy to analyze as our earlier response function, it has the important advantage of being fully self-consistent physically, in the sense that it complies with certain positivity criteria which we discuss in detail in Sec III.

With this response function, Eq. (7) reduces to (see Appendix for details),

$$\langle \Delta x^2 \rangle = \frac{2\mu}{\beta} t_{th} \left\{ \ln \left[ 2 \sinh\left(\frac{t}{t_{th}}\right) \right] + \psi^0 \left(1 + \frac{t_{th}}{2\tau}\right) + \gamma + \frac{2\tau}{t_{th}} \left[ {}_2F_1 \left(1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2t}{t_{th}}}\right) - 1 \right] \right\} \quad (9)$$

Here,  $\gamma \approx 0.5772$  is the Euler-Mascheroni constant,  $\psi^0$  is a Polygamma function of order zero, and  ${}_2F_1$  is a Hypergeometric Function (see Appendix).

In Eq. (9), the Polygamma function and the Hypergeometric function are always positive, but as  $t \rightarrow 0$ , the logarithm goes negative. This, however, is counterbalanced by the Hypergeometric function, resulting in a net positive value of the mean square displacement. We have checked this semi-analytically and found that the R.H.S of Eq. (9) is always positive. Our newer response function thus passes this consistency test. (See Fig. 1 where we have plotted  $\langle \Delta x^2 \rangle$  against time over a large range of time scales using Eq. (9).)

We can identify several different limiting cases or ‘‘regimes’’, depending on the three time scales:  $\tau =$  relaxation time,  $t_{th} =$  thermal time, and  $t =$  observation time. The thermal time  $t_{th}$  is related to the temperature  $T$  by  $\beta\hbar = \frac{\hbar}{k_B T}$ . Depending on these time scales there can be six distinct possibilities, which we will now discuss.

In Ref. [5], the cases we will call 1, 2, and 3 were studied and analytical forms for the mean square displacement were discussed for a cruder step-function form of response function,  $R(t) = \mu\theta(t - \tau)$ . Using the more

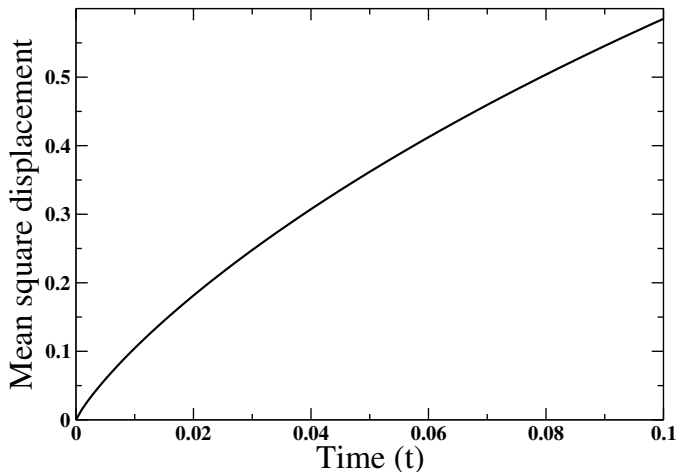


FIG. 2: Plot of the mean square displacement as a function of time in arbitrary units, under the condition,  $t \ll \tau \ll t_{th}$ . The mean square displacement is obtained from Eq. (10). In this case, the relaxation time is taken to be  $\tau = 1$  and the thermal time is taken to be  $t_{th} = 10$ .

realistic response function of Eq. (8), it is possible to get analytical forms for the other three cases as well (cases A,B, and C).

**Case A:**  $t \ll \tau \ll t_{th}$

In this limit, using Eq. (A-15) retaining terms to first order in  $t$ , and Eq. (A-19), Eq. (9) reduces to,

$$\langle \Delta x^2 \rangle = \frac{2\mu}{\beta} \left\{ \frac{t_{th}t}{\tau} \left[ 1 - \ln \left( \frac{t}{\tau} \right) - \gamma + \frac{\tau}{t_{th}} \right] \right\} \quad (10)$$

In Fig. 2, we have plotted the mean square displacement as a function of time using Eq. (10). It is possible to estimate the order of magnitude for the time and the temperature in this regime. Considering the relaxation time for sodium [7] to be  $\tau = 10\mu s$ ,  $t$  turns out to be a few  $ns$  and  $T$  is of the order of  $\mu K$ .

**Case B:**  $t \ll t_{th} \ll \tau$

In this limit, using Eq. (A-15) retaining terms to first order in  $t$ , and Eq. (A-20), Eq. (9) reduces to,

$$\langle \Delta x^2 \rangle = \frac{2\mu}{\beta} \left\{ \frac{t_{th}t}{\tau} \left[ 1 - \ln \left( \frac{2t}{t_{th}} \right) - \frac{\pi^2 t_{th}}{12\tau} + \frac{\tau}{t_{th}} \right] \right\} \quad (11)$$

In Fig. 3, we have plotted the mean square displacement as a function of time using Eq. (11). In this case, considering the same relaxation time, i.e.  $\tau = 10\mu s$ , the observation time can be estimated to be of the order of a few  $ns$  and the temperature of the order of a few  $\mu K$  to  $mK$ .

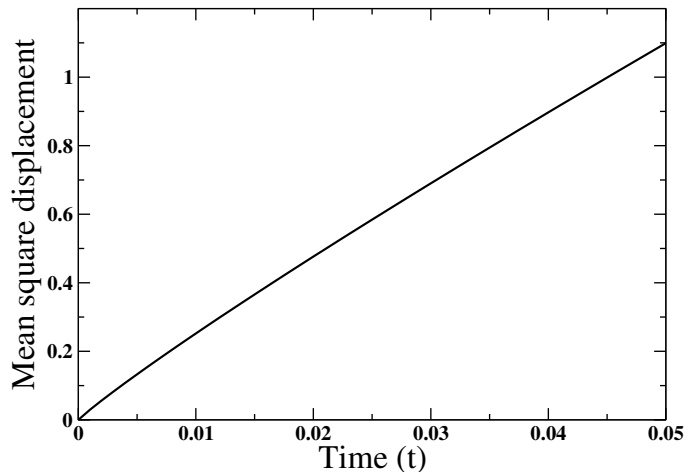


FIG. 3: Plot of the mean square displacement as a function of time in arbitrary units, under the condition,  $t \ll t_{th} \ll \tau$ . The mean square displacement is obtained from Eq. (11). In this case, the relaxation time is taken to be  $\tau = 1$  and the thermal time is taken to be  $t_{th} = 0.1$ .

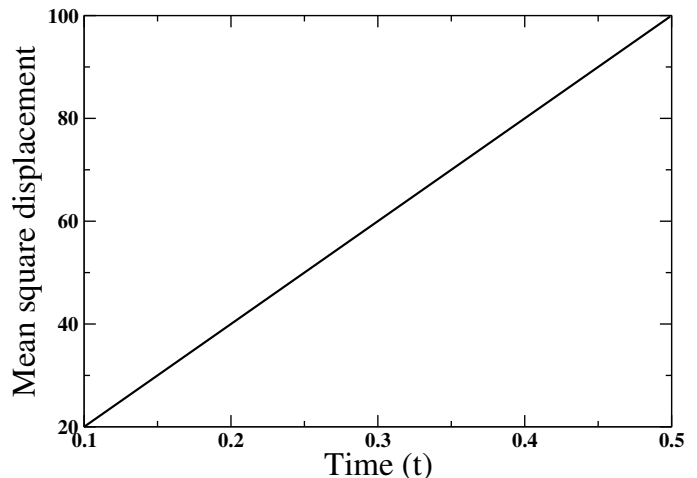


FIG. 4: Plot of the mean square displacement as a function of time in arbitrary units, under the condition,  $t_{th} \ll t \ll \tau$ . The mean square displacement is obtained from Eq. (12). In this case, the relaxation time is taken to be  $\tau = 1$  and the thermal time is taken to be  $t_{th} = 0.01$ .

**Case C:**  $t_{th} \ll t \ll \tau$

In this limit using Eq. (A-9), Eq. (A-10) and Eq. (A-20), Eq. (9) reduces to,

$$\langle \Delta x^2 \rangle = \frac{2\mu}{\beta} \left\{ t + \frac{\pi^2 t_{th}^2}{12\tau} \right\} \quad (12)$$

In Fig. 4, we have plotted the mean square displacement as a function of time using Eq. (12). In this case, considering the same relaxation time, i.e.  $\tau = 10\mu s$ , the observation time can be estimated to be of the order of a few  $ns$  to a few  $\mu s$  and the temperature of the order of a few  $mK$  to  $1K$ .

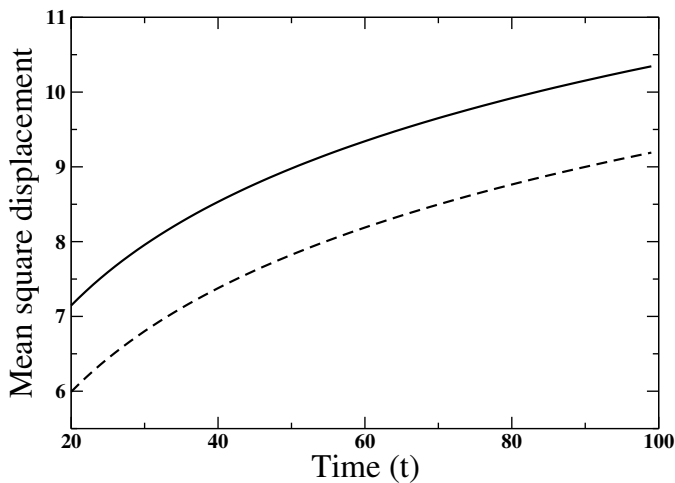


FIG. 5: Plots of the mean square displacement as a function of time under the condition,  $\tau \ll t \ll t_{th}$ . The solid line is the mean square displacement using Eq. (13), and the dashed line is the mean square displacement using Eq. (14). In this case, the relaxation time is taken to be  $\tau = 1$  and the thermal time is taken to be  $t_{th} = 100$ .

#### Case 1: Quantum regime

In the quantum limit, i.e.,  $\tau \ll t \ll t_{th}$ , using Eq. (A-11) and Eq. (A-20), Eq. (9) reduces to,

$$\langle \Delta x^2 \rangle = \frac{2\mu}{\beta} t_{th} \left\{ \ln \left( \frac{t}{\tau} \right) + \gamma \right\} \quad (13)$$

For comparison, with the step function response function, the mean square displacement in the quantum domain was [5],

$$\langle \Delta x^2 \rangle = \frac{2\mu}{\beta} t_{th} \ln \left( \frac{t}{\tau} \right) \quad (14)$$

In Fig. 5, we have plotted the mean square displacement as a function of time, in the quantum domain. The two curves are obtained using Eq. (13) for the newer response function and Eq. (14) for the step-function response function. The two curves qualitatively show the same logarithmic behaviour. But we notice a quantitative difference as manifested in a difference in the size of the intercept.

In this case, considering the same relaxation time, i.e.  $\tau = 10\mu s$ , the observation time can be estimated to be of the order of a few  $ms$  and temperatures of a few  $nK$  or below. Reaching this temperature regime seems possible with present experimental techniques in cold atom experiments where temperatures down to  $500pK$  can be reached [8].

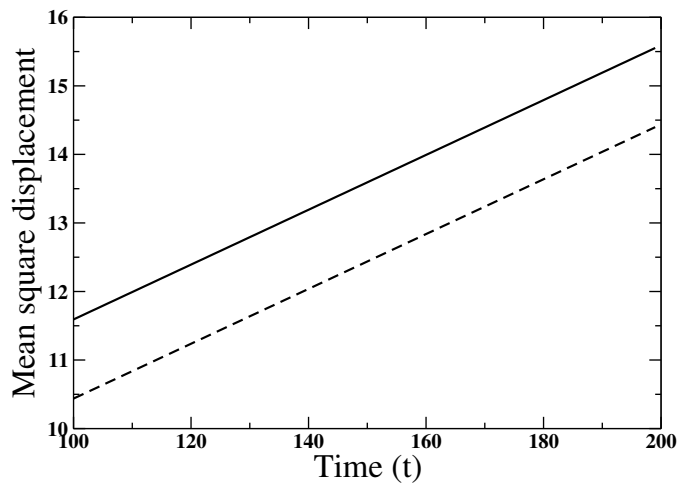


FIG. 6: Plot of the mean square displacement as a function of time in arbitrary units, under the condition,  $\tau \ll t_{th} \ll t$ . As in Fig. 5, the solid line is the mean square displacement using Eq. (15) and the dashed line is the mean square displacement using Eq. (16). In this case, the relaxation time is taken to be  $\tau = 1$  and the thermal time is taken to be  $t_{th} = 50$ .

#### Case 2: Intermediate regime

In the intermediate time regime, i.e.,  $\tau \ll t_{th} \ll t$ , using Eq. (A-11), Eq. (A-12) and Eq. (A-20), Eq. (9) reduces to,

$$\langle \Delta x^2 \rangle = \frac{2\mu}{\beta} \left\{ t + t_{th} \left[ \ln \left( \frac{t_{th}}{2\tau} \right) + \gamma \right] \right\} \quad (15)$$

Using the step-function response function, the mean square displacement in the intermediate time domain was [5],

$$\langle \Delta x^2 \rangle = \frac{2\mu}{\beta} \left\{ t + t_{th} \ln \left( \frac{t_{th}}{2\tau} \right) \right\} \quad (16)$$

In Fig. 6, we have shown the plot of the mean square displacement in the intermediate time regime. The two curves are obtained using Eq. (15) for the newer response function and Eq. (16) using step-function response function. As in Case 1 we notice that the two curves show the same qualitative behaviour. There is, however, a quantitative difference which is captured by the size of the intercept, as we noticed in Case 1.

In this case, considering the same relaxation time, i.e.  $\tau = 10\mu s$ , the observation time can be estimated to be of the order of a few  $ms$  and the temperature of the order of a few  $nK$  to  $\mu K$ . This regime can be easily realized with ultra cold atoms where the typical relaxation times can be around a few  $\mu s$  and temperature regime of  $10\mu K$  can be reached using laser cooling and a few tens of  $nK$  can be reached using evaporative cooling in optical [9] or magnetic traps [10] or Raman side-band cooling in optical lattices [11].

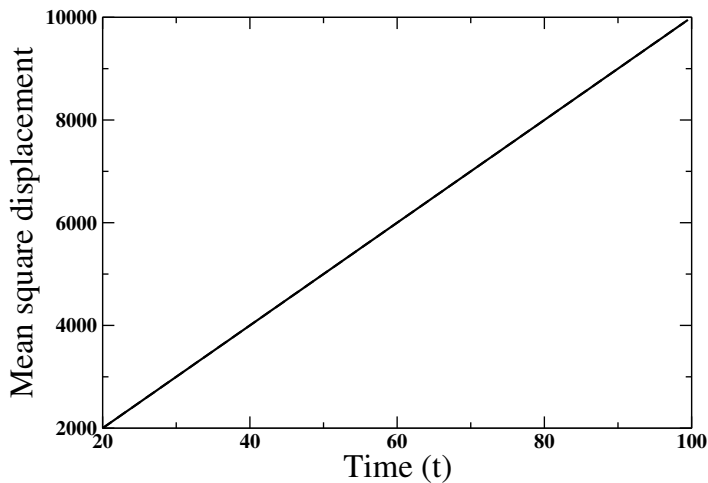


FIG. 7: Plot of the mean square displacement as a function of time in arbitrary units, under the condition,  $t_{th} \ll \tau \ll t$ . The curve is obtained by using Eq. (17). In this case, the relaxation time is taken to be  $\tau = 1$  and the thermal time is taken to be  $t_{th} = 0.02$ .

### Case 3: Classical regime

In the classical limit, i.e.,  $t_{th} \ll \tau \ll t$ , using Eq. (A-9) and Eq. (A-10), Eq. (9) reduces to,

$$\langle \Delta x^2 \rangle = \frac{2\mu}{\beta} t_{th} \left\{ \ln \left[ e^{\frac{t}{t_{th}}} \right] \right\} = \frac{2\mu}{\beta} t \quad (17)$$

Using the step-function response-function, the mean square displacement in the classical domain was [5] the same as in Eq. (17). In Fig. 7, we have shown the plot of the mean square displacement in the classical domain. Both the newer response function and the step-function response function yield the same curve.

In this case, considering the same relaxation time, i.e.  $\tau = 10\mu s$ , the observation time can be estimated to be of the order of a few *ms* to a few *s* and the temperature of the order of a few  $\mu K$  to  $mK$ .

One sees in the figures that the mean square displacement  $\langle \Delta x^2 \rangle$  is positive in all six cases.

### III. POSITIVITY CONDITIONS

In Ref. [5] we had noticed that the expression for the mean square displacement gets to be self-contradictory in a time-regime  $t \approx \tau$ . This stemmed from the fact that the response function contemplated there did not satisfy certain positivity requirements which we elaborate in this section.

The first such requirement is Wightman positivity, which one could think of as a strengthened form of positivity of the mean square displacement. The (two-point) Wightman function  $W(t)$  is defined as,

$$W(t) = \langle x(t)x(0) \rangle \quad (18)$$

Wightman positivity requires it to be of positive type (also called “positive definite”), which is equivalent to positivity of the Fourier transform:  $\widetilde{W}(\nu) > 0$ .

Using the alternative (KMS-like) form of the FDT,

$$\widetilde{W}(-\nu) = e^{2\pi\beta\hbar\nu} \widetilde{W}(\nu), \quad (19)$$

one can write for the Wightman function in the frequency domain,

$$\widetilde{W}(\nu) = \frac{1}{1 - e^{2\pi\beta\hbar\nu}} (\widetilde{W}(\nu) - \widetilde{W}(-\nu)) \quad (20)$$

The response function defined in Eq. (2) can, for  $t > 0$ , be expressed in terms of the Wightman function:

$$R(t) = \frac{i}{\hbar} (W(t) - W(-t))$$

or,  $W(t) - W(-t) = -i\hbar R(t)$

Therefore we have for all  $t$ , and for the equivalent odd function  $\check{R}(t)$  of Eq. (4)

$$W(t) - W(-t) = -i\hbar \check{R}(t)$$

or in the frequency domain,

$$\widetilde{W}(\nu) - \widetilde{W}(-\nu) = i\hbar \check{\check{R}}(\nu) \quad (21)$$

Using Eqs. (20) and (21), one can express  $\widetilde{W}(\nu)$  in terms of  $\check{\check{R}}(\nu)$  as follows:

$$\widetilde{W}(\nu) = \frac{i\hbar}{1 - e^{2\pi\beta\hbar\nu}} \check{\check{R}}(\nu) \quad (22)$$

The Wightman function  $W(t)$  is therefore of positive type if and only if the R.H.S of (22) is positive for every  $\nu$ .

Let us verify Wightman positivity for the response function of Eq. (8),  $R(t) = \mu \left( 1 - e^{-\frac{t}{\tau}} \right) \theta(t)$ . We have then, for  $t > 0$ ,

$$\begin{aligned} \check{\check{R}}(t) &= \mu \left[ \text{sgn}(t) \left( 1 - e^{-\frac{|t|}{\tau}} \right) \right] \\ &= \mu \left[ \text{sgn}(t) - \theta(t) e^{-\frac{t}{\tau}} + \theta(-t) e^{\frac{t}{\tau}} \right] \end{aligned} \quad (23)$$

Therefore,

$$\begin{aligned}
i\tilde{R}(\nu) &= \mu \left[ i \int_{-\infty}^{\infty} dt e^{2\pi i \nu t} \text{sgn}(t) - i \int_{-\infty}^{\infty} dt e^{2\pi i \nu t} \theta(t) e^{-\frac{t}{\tau}} \right. \\
&\quad \left. + i \int_{-\infty}^{\infty} dt e^{2\pi i \nu t} \theta(-t) e^{\frac{t}{\tau}} \right] \\
&= \mu \left[ i \int_0^{\infty} dt (e^{2\pi i \nu t} - e^{-2\pi i \nu t}) - i \int_0^{\infty} dt (e^{2\pi i \nu t} \right. \\
&\quad \left. - e^{-2\pi i \nu t}) e^{-\frac{t}{\tau}} \right] \\
&= \mu \left[ -2\text{Im} \int_0^{\infty} dt e^{2\pi i \nu t} + 2\text{Im} \int_0^{\infty} dt e^{(2\pi i \nu t) - \frac{t}{\tau}} \right] \\
&= \mu \left[ -2\text{Im} \left( \frac{1}{2} \delta(\nu) + \frac{i}{2\pi\nu} \right) + 2\text{Im} \frac{1}{\left(\frac{1}{\tau} - (2\pi i \nu)\right)} \right] \\
&= \mu \left[ \frac{-2}{2\pi\nu} + 2\text{Im} \frac{\frac{1}{\tau} + 2\pi i \nu}{\frac{1}{\tau^2} + (2\pi\nu)^2} \right] \\
&= \frac{4\pi\nu\mu}{\frac{1}{\tau^2} + (2\pi\nu)^2} - \frac{2\mu}{2\pi\nu} \\
&= \frac{-\mu \frac{1}{\tau^2}}{\pi\nu \left(\frac{1}{\tau^2} + (2\pi\nu)^2\right)}
\end{aligned}$$

Hence,

$$\begin{aligned}
\tilde{W}(\nu) &= \left( \frac{\hbar}{1 - e^{2\pi\beta\hbar\nu}} \right) \frac{-\mu \frac{1}{\tau^2}}{\pi\nu \left(\frac{1}{\tau^2} + (2\pi\nu)^2\right)} \\
&= \frac{\hbar\mu}{\pi\nu (e^{2\pi\beta\hbar\nu} - 1) (1 + (2\pi\nu\tau)^2)} \quad (24) \\
&\geq 0 \quad (25)
\end{aligned}$$

Therefore this response function satisfies Wightman positivity.

The second positivity requirement is passivity, which, at linear order, can be stated as follows [13, 14]. The mean work done on the system is given at this order by,

$$\bar{W} = \int dt f(t) \langle \dot{x}(t) \rangle \quad (26)$$

where  $f(t)$  is a weak perturbing force applied to the displacement  $x(t)$ . Passivity is then the requirement,

$$\bar{W} \geq 0 \quad (27)$$

(We have used the notation  $\bar{W}$  for work to distinguish it from the Wightman function  $W$ .)

By definition of the response function, we have

$$\langle x(t) \rangle - \langle x(0) \rangle = \int dt' R(t-t') f(t') \quad (28)$$

Hence the expression for work reduces to,

$$\bar{W} = \int_{-\infty}^{\infty} dt f(t) \frac{d}{dt} \left\{ \int_{-\infty}^{\infty} dt' R(t-t') f(t') \right\} \quad (29)$$

$$= \int_{-\infty}^{\infty} dt f(t) K(t-t') f(t') dt', \quad (30)$$

where  $K(t)$  is the time derivative of the position response function  $R(t)$ , i.e. the response function for the velocity. Taking Fourier transforms, and using the fact that both  $\tilde{K}$  and  $\tilde{f}$  are Fourier transforms of real functions, we can write,

$$\begin{aligned}
\bar{W} &= \int_{-\infty}^{\infty} dt f(t) \int_{-\infty}^{\infty} dt' f(t') \\
&\quad \int_{-\infty}^{\infty} d\nu e^{2\pi i \nu (t-t')} \tilde{K}(\nu)^* \\
&= \int_{-\infty}^{\infty} d\nu \tilde{K}(\nu)^* \int_{-\infty}^{\infty} dt e^{2\pi i \nu t} f(t) \\
&\quad \int_{-\infty}^{\infty} dt' e^{-2\pi i \nu t'} f(t') \\
&= \int_{-\infty}^{\infty} d\nu \tilde{K}(\nu) |\tilde{f}(\nu)|^2 \\
&= 2 \int_0^{\infty} d\nu \text{Re} \tilde{K}(\nu) |\tilde{f}(\nu)|^2
\end{aligned}$$

Since this must be positive for arbitrary (real)  $f(t)$ , passivity at linear order reduces to the positivity of the real part of the Fourier-transformed velocity-response function:

$$\text{Re} \tilde{K}(\nu) \geq 0 \quad (31)$$

One might wonder why passivity concerns only the real part of  $\tilde{K}$  whereas Wightman positivity requires that the full Fourier transform  $\tilde{W}$  be non-negative. The difference is that passivity requires positivity only for real force-functions  $f$ , whereas Wightman positivity requires that  $f^* W f$  be positive for arbitrary complex functions  $f(t)$ . If we treat  $W(t-t')$  and  $K(t-t')$  formally as matrices then, because  $f K f = f K^T f$  ( $K^T$  being the transpose), only the symmetric part of  $K$  influences the work done. Positivity of the latter then equates to positivity of the Fourier transform of this symmetric part, which is exactly the real part of the Fourier transform of  $K$  itself.

Let us check that the requirement (31) is met by our response function,  $R(t) = \mu (1 - e^{-\frac{t}{\tau}}) \theta(t)$ . For this response function,

$$K(t) = \frac{d}{dt} \left\{ \mu (1 - e^{-\frac{t}{\tau}}) \theta(t) \right\} = \frac{\mu}{\tau} e^{-\frac{t}{\tau}} \theta(t)$$

The Fourier transform of  $K(t)$  is then

$$\begin{aligned}
\tilde{K}(\nu) &= \mu \int_{-\infty}^{\infty} dt e^{2\pi i \nu t} \frac{d}{dt} \left\{ (1 - e^{-\frac{t}{\tau}}) \theta(t) \right\} \\
&= \mu \frac{\frac{1}{\tau}}{\frac{1}{\tau} - 2\pi i \nu}, \quad (32)
\end{aligned}$$

The real part of this is

$$\frac{\mu}{1 + (2\pi\nu\tau)^2}, \quad (33)$$

which is indeed non-negative for all  $\nu$ .

Our response function thus satisfies both positivity conditions. This is to be contrasted with the case of the step function response function [5]  $R(t) = \mu\theta(t - \tau)$  where positivity fails in the limit  $t \rightarrow \tau$ .

### Positivity and the FDT

The conditions for Wightman positivity and passivity are related by the FDT in its different guises, (1) and (19). By combining these with the equation,  $K = dR/dt$ , one can relate  $\widetilde{W}(\nu)$  to the real part of  $\widetilde{K}(\nu)$ , as follows.

Let us begin with  $\text{Re}\widetilde{K}(\nu)$ . Because differentiation in the time-domain corresponds to multiplication by  $i\nu$  in the frequency-domain, we can trade  $\text{Re}\widetilde{K}(\nu)$  for  $\text{Im}\widetilde{R}(\nu)$ . The latter however, is equivalent by (1) to  $\widetilde{C}(\nu)$ , which in turn is by definition half of  $\widetilde{W}(\nu) + \widetilde{W}(-\nu)$ . Then with the help of (19), we can eliminate  $\widetilde{W}(-\nu)$  from this sum to be left with a simple multiple of  $\widetilde{W}(\nu)$ . Following these steps, one finds straightforwardly that

$$\text{Re}\widetilde{K}(\nu) = \pi\nu (\exp\{2\pi\beta\nu\} - 1) \widetilde{W}(\nu), \quad (34)$$

which makes it evident that  $\text{Re}\widetilde{K}(\nu)$  is positive if and only if  $\widetilde{W}(\nu)$  is positive (where we ignore, if need be, the special case  $\beta\nu = 0$ ). Thus Wightman positivity implies linear-order passivity and conversely, as a consequence of the FDT.

**REMARK:** The requirement of Wightman positivity is quite general. Because it merely reflects the positivity of the Hilbert space inner product, it applies to any system whose description conforms to the quantum formalism based on Hilbert space. The requirement of passivity on the other hand, reflects a very special property of systems in thermal equilibrium, namely that one cannot extract work from them by purely mechanical means. It is therefore noteworthy that we have here derived passivity simply from Wightman positivity and the FDT. This indicates that the latter manages to encapsulate a surprisingly large part of the meaning of thermal equilibrium.

## IV. CONCLUSION

In this paper, proceeding solely on the basis of the fluctuation-dissipation theorem (FDT) and a choice of functional form for the response-function  $R$ , we have analysed the growth of mean square displacement as a function of time  $t$ . The response-function we have used depends on two parameters, a “mobility”  $\mu$  and a “relaxation-time”  $\tau$ , and correspondingly one encounters six different regimes defined by the ordering among the numbers,  $t$ ,  $\tau$ , and the thermal-time  $t_{th} = \beta\hbar/\pi$ . (The mobility enters only as an overall prefactor.)

One encounters in all, three qualitatively different growth-laws, which could be termed “classical”, “quantum” and “intermediate”. When  $t \gg t_{th}$ , one recovers the linear growth familiar from classical diffusion driven by thermal fluctuations. When, on the other hand,  $t \ll t_{th}$  but  $t \gg \tau$ , one is in the properly quantum regime of logarithmic growth driven by quantum fluctuations. Intermediate between these cases is one where  $t$  falls below both  $\tau$  and  $t_{th}$  and one encounters an intermediate growth proportional to  $t \ln t$ .

In an earlier study [5], the response function was chosen to be a simple step function. Such a function works well for times longer than the relaxation-time, but for very short times, it leads to inconsistencies stemming from the fact that the step function violates certain positivity conditions that a putative response function must satisfy, namely *Wightman positivity* (which trivially guarantees positivity of the mean-square displacement) and the thermodynamic condition of *passivity*.

In this connection we have exhibited some relationships among the positivity conditions in question, most importantly that (for a weak perturbing force) Wightman positivity also implies passivity when combined with the FDT. Indeed, we have shown that in the presence of the FDT, linear-order passivity is equivalent to Wightman positivity.

The response function used in our present study has a twofold advantage. Firstly, it has a form which is closer to one realizable in a cold-atom laboratory. Secondly, it satisfies the physically mandated positivity requirements and therefore gives theoretically consistent results in the entire time domain. This has allowed us to go beyond Ref. [5] in probing the short-time regime where  $t \ll \tau$ . On the other hand, in what we have called the quantum regime, we find qualitatively the same logarithmic growth as earlier, suggesting that this behavior is robust. (This is not to say, however, that there are not quantitatively distinct predictions.)

*Experimental Prospects:* The quantum law of diffusion predicted by our analysis can be tested in experiments with ultra-cold atoms [6–11, 15]. In recent years there has been considerable development in this area, and one can now hope to probe the growth of mean square displacement as a function of time in the time-temperature domains discussed here. For example using sub-Doppler cooling in optical molasses it is possible to achieve temperatures of the order of 10 micro Kelvin [7] using laser cooling techniques. With this technique, the atoms are cooled and confined in a very small region of space thanks to damping of atomic velocities. Within the confined region, the atomic motion is analogous to that of a Brownian particle. Furthermore the technique of evaporative cooling in conservative traps [6] can reach temperatures of the order of 10 nano Kelvin.

Since the various time-temperature regimes discussed in this paper all appear to be realizable in cold-atom laboratories, we are optimistic that experiments in the quantum and intermediate regimes will be performed soon,

perhaps by an experimental group with whom we have discussed our results.

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## VI. APPENDIX: DETAILS OF CALCULATIONS

Substituting  $R(t')$  from Eq. (8) in Eq. (7), we get,

$$\begin{aligned} \langle \Delta x^2 \rangle &= \frac{\mu}{\beta} \int_0^\infty dt' (1 - e^{-\frac{t'}{\tau}}) \left\{ 2 \coth \left( \frac{t'}{t_{th}} \right) \right. \\ &\quad \left. - \coth \left( \frac{t'+t}{t_{th}} \right) - \coth \left( \frac{t'-t}{t_{th}} \right) \right\} \\ &= \lim_{\epsilon \rightarrow 0} (I_1 - I_2) \end{aligned} \quad (\text{A-1})$$

$$\begin{aligned} I_1 &= \frac{\mu}{\beta} \int_\epsilon^\infty dt' \left\{ 2 \coth \left( \frac{t'}{t_{th}} \right) - \coth \left( \frac{t'+t}{t_{th}} \right) \right. \\ &\quad \left. - \coth \left( \frac{t'-t}{t_{th}} \right) \right\} \\ &= \lim_{t_\infty \rightarrow \infty} \frac{\mu}{\beta} t_{th} \left\{ 2 \ln \left[ \sinh \left( \frac{t'}{t_{th}} \right) \right] - \ln \left[ \sinh \left( \frac{|t'+t|}{t_{th}} \right) \right] \right. \\ &\quad \left. - \ln \left[ \sinh \left( \frac{|t'-t|}{t_{th}} \right) \right] \right\}_\epsilon^{t_\infty} \\ &= \frac{2\mu}{\beta} t_{th} \ln \left[ \frac{\sqrt{\sinh \left( \frac{|t+\epsilon|}{t_{th}} \right) \sinh \left( \frac{|t-\epsilon|}{t_{th}} \right)}}{\sinh \left( \frac{\epsilon}{t_{th}} \right)} \right] \\ &= \frac{2\mu}{\beta} t_{th} \ln \left[ \frac{\sinh \left( \frac{t}{t_{th}} \right)}{\sinh \left( \frac{\epsilon}{t_{th}} \right)} \right] \end{aligned} \quad (\text{A-2})$$

using,  $t \ll t_\infty$ .

$$\begin{aligned} I_2 &= \frac{\mu}{\beta} \int_\epsilon^\infty dt' e^{-\frac{t'}{\tau}} \left\{ 2 \coth \left( \frac{t'}{t_{th}} \right) - \coth \left( \frac{t'+t}{t_{th}} \right) \right. \\ &\quad \left. - \coth \left( \frac{t'-t}{t_{th}} \right) \right\} \end{aligned} \quad (\text{A-3})$$

$$\text{Consider, } I = \int_\epsilon^\infty dt' e^{-\frac{t'}{\tau}} \coth \left( \frac{t'}{t_{th}} \right) \quad (\text{A-4})$$

Setting  $\coth \left( \frac{t'}{t_{th}} \right) = y$ , then the above integral reduces to,

$$I = -t_{th} \int_{y_0}^1 dy \left( \frac{y-1}{y+1} \right)^{\frac{t_{th}}{2\tau}-1} \frac{y}{(y+1)^2} \quad (\text{A-5})$$

where,  $y_0 = \coth \left( \frac{\epsilon}{t_{th}} \right)$ . Now, if we substitute,  $(y-1)/(y+1) = zx$ , such that,  $z = (y_0-1)/(y_0+1) = e^{-\frac{2\epsilon}{t_{th}}}$ , then this integral reduces to,

$$I = -z^{\frac{t_{th}}{2\tau}} t_{th} \int_0^1 dx x^{\frac{t_{th}}{2\tau}-1} \left( \frac{1}{2} - \frac{1}{1-zx} \right) \quad (\text{A-6})$$

Using the integral form of Hypergeometric Function  ${}_2F_1$ ,

$${}_2F_1(a, b, c, z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 dx x^{b-1} (1-x)^{c-b-1} (1-zx)^{-a} \quad (\text{A-7})$$

we can write Eq. (A-6) as,

$$I = -\tau e^{-\frac{\epsilon}{\tau}} \left[ 1 - 2 {}_2F_1 \left( 1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2\epsilon}{t_{th}}} \right) \right] \quad (\text{A-8})$$

We use the following forms of the Hypergeometric functions in our analytical calculations:

$${}_2F_1(a, b, a, z) = (1-z)^{-b} \quad (\text{A-9})$$

$${}_2F_1(a, b, a, 0) = 1 \quad (\text{A-10})$$

$${}_2F_1(a, b, b, z) = (1-z)^{-a} \quad (\text{A-11})$$

$${}_2F_1(a, b, b, 0) = 1 \quad (\text{A-12})$$

Similarly, we can evaluate the other integrals in Eq. (A-3) and get,

$$\begin{aligned} I_2 &= \frac{2\mu\tau}{\beta} e^{-\frac{\epsilon}{\tau}} \left[ 2 {}_2F_1 \left( 1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2\epsilon}{t_{th}}} \right) \right. \\ &\quad \left. - 2 {}_2F_1 \left( 1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2(t+\epsilon)}{t_{th}}} \right) \right. \\ &\quad \left. - 2 {}_2F_1 \left( 1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2(t-\epsilon)}{t_{th}}} \right) \right] \\ &= \frac{4\mu\tau}{\beta} \left[ 2 {}_2F_1 \left( 1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2\epsilon}{t_{th}}} \right) \right. \\ &\quad \left. - 2 {}_2F_1 \left( 1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2t}{t_{th}}} \right) \right] \end{aligned} \quad (\text{A-13})$$

Therefore using Eqs. (A-2) and (A-13), mean square displacement can be written as,

$$\begin{aligned} \langle \Delta x^2 \rangle &= \lim_{\epsilon \rightarrow 0} \frac{2\mu}{\beta} t_{th} \left\{ \ln \left[ \frac{\sinh \left( \frac{t}{t_{th}} \right)}{\sinh \left( \frac{\epsilon}{t_{th}} \right)} \right] \right. \\ &\quad \left. - \frac{2\tau}{t_{th}} \left[ 2 {}_2F_1 \left( 1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2\epsilon}{t_{th}}} \right) \right. \right. \\ &\quad \left. \left. - 2 {}_2F_1 \left( 1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2t}{t_{th}}} \right) \right] \right\} \end{aligned} \quad (\text{A-14})$$



In this expression for mean square displacement, the logarithmic and Hypergeometric functions of  $\epsilon$  diverge, when  $\epsilon \rightarrow 0$ . These divergences cancel if we expand the Hypergeometric Function for small  $\epsilon$ :

$$\begin{aligned}
& {}_2F_1\left(1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2\epsilon}{t_{th}}}\right) \\
& \approx -\frac{t_{th}}{2\tau} \left( \psi^{(0)}\left(\frac{t_{th}}{2\tau}\right) + \ln\left(\frac{2\epsilon}{t_{th}}\right) + \gamma \right) \\
& - \frac{\epsilon t_{th}}{2\tau^2} \left( -\frac{\tau}{t_{th}} + \psi^0\left(1 + \frac{t_{th}}{2\tau}\right) + \ln\left(\frac{2\epsilon}{t_{th}}\right) + \gamma - 1 \right) \\
& - \frac{\epsilon^2 t_{th}}{24\tau^3} \left( \frac{2\tau^2}{t_{th}^2} - 6\frac{\tau}{t_{th}} + 6\psi^0\left(1 + \frac{t_{th}}{2\tau}\right) \right) \\
& + 6 \ln\left(\frac{2\epsilon}{t_{th}}\right) + 6\gamma - 9 + O(\epsilon^3) + \dots
\end{aligned} \tag{A-15}$$

where,  $\psi^0(x)$  is Polygamma function of order zero and  $\gamma$  is Euler-Mascheroni constant. The last step used the relations,

$$\psi^0(x) = x \sum_{n=1}^{\infty} \frac{1}{n(n+x)} - \frac{1}{x} - \gamma \tag{A-16}$$

Substituting Eq. (A-15) in Eq. (A-14), we get finally,

$$\begin{aligned}
\langle \Delta x^2 \rangle = & \frac{2\mu}{\beta} t_{th} \left\{ \ln \left[ 2 \sinh \left( \frac{t}{t_{th}} \right) \right] + \psi^0 \left( 1 + \frac{t_{th}}{2\tau} \right) + \gamma + \right. \\
& \frac{2\tau}{t_{th}} \left[ {}_2F_1 \left( 1, \frac{t_{th}}{2\tau}, 1 + \frac{t_{th}}{2\tau}, e^{-\frac{2t}{t_{th}}} \right) \right. \\
& \left. \left. - 1 \right] \right\}
\end{aligned} \tag{A-17}$$

using the identity:

$$\psi^0(1+x) = \psi^0(x) + \frac{1}{x} \tag{A-18}$$

The asymptotic forms of  $\psi^0(1+x)$  are:

$$\psi^0(1+x) = \ln(x), \quad x \gg 1 \tag{A-19}$$

$$\psi^0(1+x) = -\gamma + \frac{\pi^2}{6}x, \quad x \ll 1 \tag{A-20}$$

We have used these asymptotic limits in our analytical calculations.

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