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Normalization of collisional decoherence: squaring the delta function, and an independent cross-check

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Abstract

We show that when the Hornberger–Sipe calculation of collisional decoherence is carried out with the squared delta function a delta of energy, instead of a delta of the absolute value of momentum, following a method introduced by Diósi, the corrected formula for the decoherence rate is simply obtained. The results of Hornberger and Sipe and of Diósi are shown to be in agreement. As an independent cross-check, we calculate the mean squared coordinate diffusion of a hard sphere implied by the corrected decoherence master equation, and show that it agrees precisely with the same quantity as calculated by a classical Brownian motion analysis.

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1. Introduction

The calculation of collisional decoherence was initiated by Joos and Zeh [1], with generalizations of their result and corrections to the overall normalization given in papers of Gallis and Fleming [2], Dodd and Halliwell [3], and Hornberger and Sipe [4]. An even more general calculation of collisional decoherence was also given by Diósi [5], but this was not known to Hornberger and Sipe, while noted by Dodd and Halliwell, as well as in the master equation papers of Altenmüller, Müller and Schenzle [6] and of Vacchini [7]. A difficulty encountered in [1, 2, 4] is the appearance of a squared delta function of the absolute value of momentum in the calculation of the decoherence rate. To circumvent this, Hornberger and Sipe carried out a careful wave packet analysis, which gives an answer smaller by a factor of 2π than that given by Gallis and Fleming, and this result is in agreement with experiment [8].

In the course of an alternative derivation of the corrected result, following the ‘traditional approach’ of [1, 2], Hornberger and Sipe introduce a rule in which the squared delta function of the absolute value of momentum is evaluated in terms of an *inverse* scattering cross section, which drops out later in their calculation. This mixing of kinematic quantities (such as a

squared delta function) and dynamical ones (such as a cross section) is unconventional, and Hornberger and Sipe describe this part of their calculation as speculative. In section 2 we show that an entirely conventional completion of the Hornberger–Sipe calculation is possible, if one follows the method used in the earlier and more general master equation derivation given by Diósi, and also used in the derivation of Dodd and Halliwell. These authors retain the delta function of energy that appears as the \mathcal{T} -matrix coefficient, rather than converting this delta function to a delta function of the absolute value of momentum. This makes a difference when squaring the delta function. For a squared delta function of energy, one can use the standard rule of evaluating $\delta(0)$ in terms of the elapsed conjugate time variable, as is done in the usual textbook ‘golden rule’ calculation. For a delta function of the absolute value of momentum, it is not so clear what to use as the corresponding conjugate variable when taking the square, and this appears to be the root of the difficulties in the earlier calculations of [1, 2, 4].

In section 3 we compare the Hornberger–Sipe and Diósi results and show that they are the same; hence Diósi’s 1995 calculation appears to be the first giving the correct result for the collisional decoherence rate. In section 4 we give an independent check of the corrected expression for collisional decoherence, by using the corresponding master equation to evaluate the scattering-induced translational Brownian diffusion of a hard sphere in the geometric scattering limit. Planck’s constant cancels out in this calculation, and so the result obtained this way can be directly compared with the classical Brownian diffusion of a hard sphere, and the two calculations are in precise agreement.

2. Calculation using a squared energy delta function

To keep this section concise, we will use the notation of Hornberger and Sipe, and give just a brief summary of their calculation up to the point where our treatment begins to differ from theirs. We consider a Brownian particle in a bath of N scattering particles of mass m , contained in normalization volume Ω . In the dilute case, the scatterings of the bath particles from each other can be neglected, and their scatterings from the Brownian particle are independent of one another. Then the effect of the N bath particles is obtained by considering the effect of a single bath particle, and multiplying by N at the end of the calculation. For a single scattering, the effect of the collision is to change the density matrix $\rho_0(\mathbf{R}_1, \mathbf{R}_2)$ to

$$\rho(\mathbf{R}_1, \mathbf{R}_2) = \eta(\mathbf{R}_1, \mathbf{R}_2)\rho_0(\mathbf{R}_1, \mathbf{R}_2), \quad (1)$$

with the factor $\eta(\mathbf{R}_1, \mathbf{R}_2)$ given by

$$\eta(\mathbf{R}_1, \mathbf{R}_2) = \text{tr}_{\text{bath}} \left\{ e^{-i\mathbf{p}\cdot\mathbf{R}_2/\hbar} \mathcal{S}_0^\dagger e^{i\mathbf{p}\cdot(\mathbf{R}_2-\mathbf{R}_1)/\hbar} \mathcal{S}_0 e^{i\mathbf{p}\cdot\mathbf{R}_1/\hbar} \rho^{\text{bath}} \right\}. \quad (2)$$

Here \mathcal{S}_0 is the scattering matrix, and ρ^{bath} corresponds to an ensemble momentum space weighting

$$\int d\mathbf{p} \mu(\mathbf{p}), \quad (3a)$$

where for a thermal ensemble with $\beta = (kT)^{-1}$ one has

$$\mu(\mathbf{p}) = \left(\frac{\beta}{2\pi m} \right)^{3/2} e^{-\beta \mathbf{p}^2/(2m)}. \quad (3b)$$

Substituting $\mathcal{S}_0 = 1 + i\mathcal{T}_0$, evaluating the bath trace in a momentum basis, inserting a complete set of intermediate states, changing from box to continuum normalization, and using the unitarity relation $i(\mathcal{T}_0 - \mathcal{T}_0^\dagger) = -\mathcal{T}_0^\dagger \mathcal{T}_0$, Hornberger and Sipe show that equation (2) takes the form

$$\eta(\mathbf{R}_1, \mathbf{R}_2) = \int d\mathbf{p} \mu(\mathbf{p}) \left[1 - \frac{(2\pi\hbar)^3}{\Omega} \int d\mathbf{p}' (1 - e^{i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{R}_1-\mathbf{R}_2)/\hbar}) |\langle \mathbf{p}' | \mathcal{T}_0 | \mathbf{p} \rangle|^2 \right]. \quad (4a)$$

This equation, which is equation (51) of Hornberger and Sipe, and without the weighting over $\mu(\mathbf{p})$ also corresponds to the first line of equation (2.11) of Gallis and Fleming, will be the starting point for our analysis.

Denoting the elapsed time in the scattering process by T , so that equations (1) and (4a) implicitly refer to time T , and recalling that $1 = \int d\mathbf{p} \mu(\mathbf{p})$, we can rewrite equations (1) and (4a) as

$$\begin{aligned} \rho(\mathbf{R}_1, \mathbf{R}_2; T) - \rho(\mathbf{R}_1, \mathbf{R}_2; 0) &= (\eta(\mathbf{R}_1, \mathbf{R}_2; T) - 1)\rho_0(\mathbf{R}_1, \mathbf{R}_2) \\ &= -\rho_0(\mathbf{R}_1, \mathbf{R}_2) \int d\mathbf{p} \mu(\mathbf{p}) \frac{(2\pi\hbar)^3}{\Omega} \int d\mathbf{p}' (1 - e^{i(\mathbf{p}-\mathbf{p}') \cdot (\mathbf{R}_1 - \mathbf{R}_2)/\hbar}) |\langle \mathbf{p}' | \mathcal{T}_0 | \mathbf{p} \rangle|^2. \end{aligned} \quad (4b)$$

Our next task will be to evaluate the squared matrix element appearing in the integrand of equation (4b).

The general \mathcal{T}_0 matrix element $\langle \mathbf{q}_2 | \mathcal{T}_0 | \mathbf{q}_1 \rangle$ can as usual be expressed in terms of the scattering amplitude $f(\mathbf{q}_2, \mathbf{q}_1)$ and an energy-conserving delta function,

$$\begin{aligned} \langle \mathbf{q}_2 | \mathcal{T}_0 | \mathbf{q}_1 \rangle &= \frac{1}{2\pi\hbar m} \delta(E_2 - E_1) f(\mathbf{q}_2, \mathbf{q}_1) \\ &= \frac{1}{2\pi\hbar q_2} \delta(q_2 - q_1) f(\mathbf{q}_2, \mathbf{q}_1). \end{aligned} \quad (5)$$

Instead of using the second line of equation (5) to form the square of the \mathcal{T}_0 matrix element, we will use the first line, using the second line only *after* the delta function of zero energy argument has been evaluated. Thus, we have

$$|\langle \mathbf{q}_2 | \mathcal{T}_0 | \mathbf{q}_1 \rangle|^2 = \frac{1}{(2\pi\hbar m)^2} \delta^2(E_2 - E_1) |f(\mathbf{q}_2, \mathbf{q}_1)|^2. \quad (6)$$

Using the Fourier representation for the energy delta function,

$$\delta(E_2 - E_1) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \exp[i(E_2 - E_1)t/\hbar], \quad (7a)$$

we find

$$\begin{aligned} \delta^2(E_2 - E_1) &= \delta(E_2 - E_1)\delta(0) \\ &= \delta(E_2 - E_1) \frac{1}{2\pi\hbar} \int dt \\ &= \delta(E_2 - E_1) \frac{T}{2\pi\hbar} \\ &= \frac{m}{q_2} \frac{T}{2\pi\hbar} \delta(q_2 - q_1), \end{aligned} \quad (7b)$$

where in the final line we have converted the energy delta function to a delta function of the absolute value of the three-momentum. Here T is the elapsed time interval, which we assume to be longer than the time for a single scattering, but still short compared to the characteristic decoherence time of the Brownian particle in the N -particle bath.

Replacing $\mathbf{q}_2, \mathbf{q}_1$ by \mathbf{p}', \mathbf{p} respectively, substituting equations (7b) and (5) into equation (4b), and writing $d\mathbf{p}' = d\hat{n}(p')^2 dp'$, with $d\hat{n}$ a solid angle differential, we can immediately integrate the delta function of the absolute value of momentum. Using

$$\frac{(2\pi\hbar)^3}{\Omega} \frac{1}{(2\pi\hbar m)^2} p'^2 \frac{m}{p} \frac{T}{2\pi\hbar} = \frac{T}{\Omega} \frac{p}{m}, \quad (8a)$$

we thus get

$$\rho(\mathbf{R}_1, \mathbf{R}_2; T) - \rho(\mathbf{R}_1, \mathbf{R}_2; 0) = -\rho_0(\mathbf{R}_1, \mathbf{R}_2) \frac{T}{\Omega} \times \int d\mathbf{p} \mu(\mathbf{p}) \frac{p}{m} \int d\hat{n} (1 - e^{i(\mathbf{p}-p\hat{n}) \cdot (\mathbf{R}_1 - \mathbf{R}_2)/\hbar}) |f(p\hat{n}, \mathbf{p})|^2. \quad (8b)$$

Multiplying by N to take account of the fact that each of the N bath particles makes a contribution equal to equation (8b), denoting the bath density N/Ω by n , dividing by T , and finally passing to the limit of small T , we get the result

$$\frac{\partial \rho(\mathbf{R}_1, \mathbf{R}_2; t)}{\partial t} = -F(\mathbf{R}_1 - \mathbf{R}_2) \rho(\mathbf{R}_1, \mathbf{R}_2; t), \quad (9a)$$

with

$$F(\mathbf{R}_1 - \mathbf{R}_2) = n \int d\mathbf{p} \mu(\mathbf{p}) \frac{p}{m} \int d\hat{n} (1 - e^{i(\mathbf{p}-p\hat{n}) \cdot (\mathbf{R}_1 - \mathbf{R}_2)/\hbar}) |f(p\hat{n}, \mathbf{p})|^2. \quad (9b)$$

This is the form of the final result for the decoherence-induced master equation given in equation (55), and in the unnumbered immediately preceding equation, of Hornberger and Sipe [4]. By defining $\nu(p)$ by

$$\mu(\mathbf{p}) d\mathbf{p} = \frac{\nu(p) dp d\hat{s}}{4\pi}, \quad (10a)$$

with $d\hat{s}$ a second solid angle differential, so that $\int_0^\infty dp \nu(p) = 1$, Hornberger and Sipe also rewrite equation (9b) in the equivalent form (after a relabelling of the integration variables)

$$F(\mathbf{R}) = n \int_0^\infty dq \nu(q) \frac{q}{m} \int \frac{d\hat{n}_1 d\hat{n}_2}{4\pi} (1 - e^{iq(\hat{n}_1 - \hat{n}_2) \cdot \mathbf{R}/\hbar}) |f(q\hat{n}_2, q\hat{n}_1)|^2. \quad (10b)$$

In the limit of large \mathbf{R} , the exponential term in equations (9b) and (10b) averages to zero provided that $\hat{n}_2 \neq \hat{n}_1$, while in the forward direction $\hat{n}_2 = \hat{n}_1$ the integrand in equations (9b) and (10b) vanishes for all \mathbf{R} . Hence one has

$$\begin{aligned} F(\mathbf{R} \rightarrow \infty) &= n \int_0^\infty dq \nu(q) \frac{q}{m} \int_{\hat{n}_2 \neq \hat{n}_1} \frac{d\hat{n}_1 d\hat{n}_2}{4\pi} |f(q\hat{n}_2, q\hat{n}_1)|^2 \\ &= n \int_0^\infty dq \nu(q) \frac{q}{m} \sigma(q), \end{aligned} \quad (10c)$$

with $\sigma(q)$ the total cross section (excluding a possible delta function contribution to the forward diffraction peak). In other words, the large \mathbf{R} asymptote of $F(\mathbf{R})$ is the thermal ensemble average $\langle n\nu\sigma \rangle_{AV}$ of the non-forward scattering rate $n(q/m)\sigma(q)$. Correspondingly, from equations (4b) and (8b), as modified by multiplication by the factor N , we see that $\eta(\mathbf{R}_1, \mathbf{R}_2; T) = 1 - TF(\mathbf{R}_1 - \mathbf{R}_2)$ has the large \mathbf{R} asymptote $\eta(\infty; T) = 1 - T\langle n\nu\sigma \rangle_{AV}$. Thus $\eta(\infty; T)$ vanishes for T equal to the inverse of the averaged non-forward scattering rate, a result reminiscent of, but not identical to, the condition $\eta(\infty) = 0$ imposed by Hornberger and Sipe on the single collision decoherence function in their equation (45), on which they base their method for evaluating the square of a delta function of the absolute value of momentum. (We emphasize, however, that in the calculation leading to equation (9b) we have not fixed T by imposing such a condition.)

3. Comparison of the Hornberger–Sipe and Diósi results

The calculation of Diósi includes effects of recoil of the Brownian particle; we show in this section that in the limit of an infinitely heavy Brownian particle, the results of Hornberger–Sipe

and of Diósi are in agreement. When recoil is neglected, Diósi's result is his equation (19), which reads

$$\frac{d\rho}{dt} = n_0 \int dE d\Omega_i d\Omega_f k^2 \frac{d\sigma(\theta, E)}{d\Omega_f} \rho^\varepsilon(\mathbf{k}_i) \left(V_{\mathbf{k}_f \mathbf{k}_i} \rho V_{\mathbf{k}_f \mathbf{k}_i}^\dagger - \frac{1}{2} \{ V_{\mathbf{k}_f \mathbf{k}_i}^\dagger V_{\mathbf{k}_f \mathbf{k}_i}, \rho \} \right). \quad (11a)$$

Substituting into equation (11a) Diósi's equation (20) (with the Brownian particle recoil term dropped),

$$V_{\mathbf{k}_f \mathbf{k}_i} = \exp(-i\mathbf{k}_{fi} \cdot \mathbf{q}) = \exp(-i(\mathbf{k}_f - \mathbf{k}_i) \cdot \mathbf{q}), \quad (11b)$$

taking the matrix element of equation (11a) between \mathbf{q} eigenstates $\langle \mathbf{R}_1 |$ and $|\mathbf{R}_2 \rangle$, and writing

$$\rho(\mathbf{R}_1, \mathbf{R}_2; t) = \langle \mathbf{R}_1 | \rho(t) | \mathbf{R}_2 \rangle, \quad (11c)$$

we get

$$\frac{d\rho(\mathbf{R}_1, \mathbf{R}_2; t)}{dt} = -n_0 \int dE d\Omega_i d\Omega_f k^2 \frac{d\sigma(\theta, E)}{d\Omega_f} \rho^\varepsilon(\mathbf{k}_i) (1 - e^{i(\mathbf{k}_i - \mathbf{k}_f) \cdot (\mathbf{R}_1 - \mathbf{R}_2)}) \rho(\mathbf{R}_1, \mathbf{R}_2; t). \quad (12)$$

Taking account of the fact that $dE = dk^2/(2m) = (k/m) dk$, together with $d\sigma(\theta, E)/d\Omega_f = |f|^2$, where f is the scattering amplitude, along with $\rho^\varepsilon(\mathbf{k}_i) = \mu(\mathbf{k}_i)$ and some obvious relabelling of variables, one sees that equation (12) is identical to equations (9a) and (9b) that follow from the analysis of Hornberger and Sipe.

Diósi also gives the expansion of equation (12) to leading order in $\mathbf{R} = \mathbf{R}_1 - \mathbf{R}_2$. Working now in the other direction, from equation (10b), the simplest way to find the leading order \mathbf{R} dependence is to note that $F(\mathbf{R})$ is a rotationally invariant function of \mathbf{R} . Hence it suffices to evaluate the average over the direction of \mathbf{R} . Expanding the exponential in equation (10b), we have

$$1 - e^{iq(\hat{n}_1 - \hat{n}_2) \cdot \mathbf{R}/\hbar} = 1 - iq(\hat{n}_1 - \hat{n}_2) \cdot \mathbf{R}/\hbar + \frac{1}{2}(q^2/\hbar^2)[(\hat{n}_1 - \hat{n}_2) \cdot \mathbf{R}]^2 + \dots \quad (13a)$$

The average of $[(\hat{n}_1 - \hat{n}_2) \cdot \mathbf{R}]^2$ over the direction of \mathbf{R} is

$$\begin{aligned} \frac{1}{3} R^2 \sum_i [(\hat{n}_1 - \hat{n}_2) \cdot \hat{i}]^2 &= \frac{1}{3} R^2 (\hat{n}_1 - \hat{n}_2)^2 \\ &= \frac{2}{3} R^2 (1 - \hat{n}_1 \cdot \hat{n}_2) = \frac{4}{3} R^2 \sin^2(\theta/2), \end{aligned} \quad (13b)$$

with θ the angle (the scattering angle) between \hat{n}_1 and \hat{n}_2 . Substituting equations (13a) and (13b) into equation (10b), we get

$$F(\mathbf{R}) = R^2 \Lambda, \quad (14a)$$

with

$$\begin{aligned} \Lambda &= \frac{2}{3} \frac{n}{\hbar^2} \int_0^\infty dq v(q) \frac{q}{m} q^2 \int \frac{d\hat{n}_1 d\hat{n}_2}{4\pi} \sin^2(\theta/2) |f(q\hat{n}_2, q\hat{n}_1)|^2 \\ &= \frac{2}{3} \frac{n}{\hbar^2} \int d\mathbf{q} \mu(\mathbf{q}) \frac{q}{m} q^2 \int d\hat{n}_2 \sin^2(\theta/2) |f(q\hat{n}_2, q\hat{n}_1)|^2. \end{aligned} \quad (14b)$$

With the shifts in notation noted above, this equation for Λ is identical to equation (22) of Diósi, which gives what he terms the diffusion parameter D_{pp} .

4. Comparison of decoherence-based and classical calculations of Brownian translational diffusion

Let us now apply the result of equations (14a) and (14b) to the quantum Brownian motion of a Brownian particle of mass M and radius a , with a large enough so that $pa \gg 1$ for important bath particle momenta. In this case, the quantum scattering differential cross section consists of two parts [9]: an isotropic part, with an integrated cross section contribution of πa^2 , and a forward diffraction peak, again contributing cross section πa^2 . Since the integrand of equation (14b) vanishes for forward scattering, the forward diffraction peak makes no contribution. Thus we can evaluate the integrals by taking the scattering amplitude to be a constant, $f(q\hat{n}_2, q\hat{n}_1) = F$, with

$$\int d\hat{s} |F|^2 = 4\pi |F|^2 = \pi a^2, \quad (15a)$$

that is, with

$$|F|^2 = a^2/4. \quad (15b)$$

Substituting into equation (14b), we then find that

$$\Lambda = \frac{n\pi a^2 \langle q^2 v \rangle_{AV}}{3\hbar^2}. \quad (16)$$

Here we have defined

$$\langle q^2 v \rangle_{AV} = \int_0^\infty dq v(q) q^2 \frac{q}{m} = 4(m/\pi)^{\frac{1}{2}} (2kT)^{\frac{3}{2}}, \quad (17a)$$

where we used the expression

$$v(q) = 4\pi q^2 \left(\frac{\beta}{2\pi m} \right)^{\frac{3}{2}} e^{-\beta q^2/(2m)}, \quad (17b)$$

which follows from the definitions of equations (3b) and (10a), to evaluate the thermal average.

Substituting equation (14a) into equation (9a), we then get

$$\frac{\partial \rho(\mathbf{R}_1, \mathbf{R}_2; t)}{\partial t} = -\Lambda (\mathbf{R}_1 - \mathbf{R}_2)^2 \rho(\mathbf{R}_1, \mathbf{R}_2; t), \quad (18a)$$

which with equation (11c) is equivalent to the operator equation

$$\frac{\partial \rho(t)}{\partial t} = -\Lambda \sum_{j=1}^3 [R_j, [R_j, \rho(t)]], \quad (18b)$$

with R_j denoting the Cartesian components of \mathbf{R} . Adding the kinetic energy term to the differential equation for $\rho(t)$, we get the total evolution equation

$$\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar} [H_{\text{kin}}, \rho(t)] - \Lambda \sum_{j=1}^3 [R_j, [R_j, \rho(t)]], \quad (19a)$$

with the kinetic Hamiltonian for the Brownian particle given by

$$H_{\text{kin}} = \sum_{j=1}^3 \frac{P_j^2}{2M}. \quad (19b)$$

Here P_j is the momentum operator corresponding to the coordinate operator R_j , so that $[R_j, P_k] = i\hbar \delta_{jk}$.

From equations (19a) and (19b), one can calculate the mean squared coordinate diffusion as a function of time, for a Brownian particle that starts at $\mathbf{R} = \mathbf{0}$ at $t = 0$ with zero drift velocity. This calculation in the one-dimensional case is given in [10], by constructing a generating function for the trace of $\rho(t)$ multiplied by an arbitrary polynomial constructed from R_j and P_k . For the mean square coordinate deviation, the result on converting to the present notation is (with no sum implied over j)

$$\langle R_j^2 \rangle = \text{tr } \rho(t) R_j^2 = \frac{2\Lambda \hbar^2 t^3}{3M^2}. \quad (20a)$$

Substituting equation (16) for Λ and equation (17a) for the thermal average of $q^2 v$, we get finally (again with j unsummed)

$$\langle R_j^2 \rangle = C(kT)^{\frac{3}{2}} n m^{\frac{1}{2}} a^2 t^3 / M^2, \quad (20b)$$

with

$$C = \frac{16}{9} (2\pi)^{\frac{1}{2}}. \quad (20c)$$

Note that the Planck constant \hbar has dropped out of this result. Hence the formula of equations (20b) and (20c) is a classical result, and should be recoverable by a purely classical calculation.

The formulae needed for a classical Brownian motion evaluation of $\langle R_j^2 \rangle$ are summarized in a recent paper by Collett and Pearle [11]. Their equation (2.2) gives (again with j unsummed)

$$\langle R_j^2 \rangle = \frac{2kT\xi t^3}{3M^2}, \quad (21a)$$

with ξ a viscosity factor, which for a sphere of radius a in a dilute bath is given by their equation (2.5),

$$\xi = \frac{8}{3} n a^2 (2\pi m k T)^{\frac{1}{2}}. \quad (21b)$$

Substituting equation (21b) into equation (21a) then gives a result identical to equations (20b) and (20c) above. Since the result of equations (20b) and (20c) is directly proportional to the normalization constant in the collisional decoherence rate, this agreement gives added confirmation of the correctness of equation (9b).

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