

Decoherence, the Density Matrix, the Thermal State and the Classical World

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Abstract Decoherence has been the basis for understanding the emergence of the classical world from its quantum underpinnings. Unfortunately the calculations establishing decoherence overshoot and, based on assumptions that break down, predict that with the passage of time the off-diagonal elements of the density matrix become arbitrarily small. It has been recognized by some authors that the thermal state, assumed to hold for systems in equilibrium, places a bound on off diagonal terms. In this article we establish—preserving the conservation of energy, as is not the case for previous work—that indeed the thermal state is an attractor under scattering. Moreover, the bound on the off-diagonal terms present in the thermal state does not contradict everyday experience.

Keywords Decoherence · Density matrix · Thermal state · Classical world

1 Introduction

The book of Giulini et al. [1] deals with some of the most fundamental questions one can ask about the world around us. The response to some of those questions is based on earlier calculations of Joos and Zeh [2,3] as well as work by Tegmark [4]. The essential feature, on which all else depends, is that the environment—meaning the myriad of tiny interactions that every observed particle experiences, makes the density matrix (ρ) of that particle nearly diagonal in coordinate space. And the longer you let your test particle interact with the environment, the more diagonal ρ becomes. There is no lower bound for the range of off-diagonal terms in coordinate space.

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As recognized by Joos and Zeh [3] these conclusions are only valid under a no-recoil assumption on the quantum scattering and are ultimately superseded. Such an assumption of course violates energy conservation. In actuality, one presumes that eventually a gas arrives at a thermal state, with a density matrix given by $\rho \sim \exp(-\beta H)$ (here β is the inverse temperature and H the total Hamiltonian). Regularizing ρ by confining the system to a finite volume, V , this implies the long-time presence of off-diagonal coordinate space matrix elements. It is presumed (but not proved as a consequence of scattering theory in [2,3]) that these off-diagonal elements must extend to distances on the order of the thermal wavelength, $\sim \hbar\sqrt{\beta/m}$. (Definitions are more precise below.) Note too that it is not clear to us whether *with* energy conservation the earlier calculations would avoid the paradox of an ever-more-diagonal density matrix.)

In the present article we prove, with one technical assumption, that under the true dynamics—not assuming zero recoil—the thermal state is an attractor. In this we assume that the bath is itself in a thermal state. Other attempts have been made to maintain energy conservation in this calculation [4] but unfortunately they are not correct, as we will explain.

2 The Thermal State

Consider the reduced one-particle density matrix for a free-particle in a gas of many particles. The temperature is T , Boltzmann's constant k_B and the inverse temperature $\beta = 1/k_B T$. The volume available is V . Although the particle is nominally designated “free” it is assumed to have small interactions with others so that it is at equilibrium (the usual story for an “ideal gas”¹). The single particle Hamiltonian is $p^2/2m$ and the density matrix²

$$\rho = \frac{1}{V} \exp(-\beta H), \text{ or } \langle x|\rho|y\rangle = \frac{1}{V} \exp\left(-\frac{m(x-y)^2}{2\beta\hbar^2}\right). \quad (1)$$

$x, y \in \mathbb{R}^3$ label the matrix ρ and as such give precise information on ρ 's off-diagonal behavior. In particular Eq. (1) shows that the drop-off as you move away from the diagonal ($x = y$) is governed by

$$\lambda = \frac{\hbar}{\sqrt{mk_B T/2}} = \frac{1}{\sqrt{\pi}} \lambda_{\text{th}}, \quad (2)$$

with λ_{th} the thermal wavelength [6]. Thus off-diagonal elements *do* decay, but have a finite distance scale. As remarked, the calculations in the cited references, by virtue of their assumptions, are unable to reach this conclusion.

¹ This equilibration is the usual fairy tale that one accepts when presenting the assumptions of statistical mechanics. We too accept it, although as we have commented when examining the notion of ergodicity [5] (see especially the response to Gaspard's comments), the foundations of physics can be considered to be “faith based.”

² Some technical issues intrude here, since the trace of $\exp(\text{const}(x-y)^2)$ is infinite if x and y are unrestricted in \mathbb{R}^3 . One can confine the system to a volume V with periodic boundary conditions. ρ is then a Jacobi theta function, and one immediately can check that except near the boundaries of the box the extra terms are negligible. Alternatively the entire system can be put in a weak harmonic oscillator potential $m\omega^2 x^2/2$ and one can take $\omega \rightarrow 0$. Again, except for large x (such that $m\omega|x|$ is significant) one recovers the result given in Eq. (1). Some of these cutoff methods will be used explicitly below.

References [2] and [3] point out that true isolation of a system from its environment is impossible. For them the shrinkage of the off-diagonal matrix elements of $\rho(\mathbf{r}, \mathbf{r}')$ is a consequence of small scatterings, which according to them and to [4], are sufficient to reduce the off-diagonal values. But one should bear in mind that the thermal wavelength has nothing to do with external scatterings (e.g., the movement of matter on the star Sirius, as mentioned by Borel [7]). It is a quantity entirely dependent on contact with a thermal reservoir at some given temperature. As a result the idea that collisions with external sources other than the heat bath ultimately lead to the thermal wavelength has not been justified.

We will show that collisions, at the given temperature, can lead to the thermal state and as a consequence to the dropoff of the off diagonal elements of the density matrix with the correct value, i.e., the thermal wavelength.

3 Formal Scattering Theory

There is a test particle, of mass M , having an initial density matrix. It is immersed in a bath of particles of mass m also possessing a so-far unspecified density matrix. The initial total density matrix is assumed to be the product. They scatter, yielding a final overall density matrix that in general has them entangled. The reduced density matrix of the test particle is the trace of the overall matrix over the bath particle coordinates and we assume that this is to be used in product form with any further interactions. This is repeated, thereby using the assumption that correlations from successive scatterings can be neglected.

Joos and Zeh [2] (see also [8]) proceeded in this fashion with one additional assumption: there is no recoil.³ They found that each successive scattering made the density matrix closer to being diagonal in coordinate space, so that with a long series of similar scatterings the approach to zero of the off-diagonal elements is exponential (in time).

The details of the proof appear to us sound, and we have checked their calculations by examining the $M \rightarrow \infty$ limit of our own calculations. Nevertheless, the *assumption* violates energy conservation. In the absence of recoil the test particle energy will tend to increase. Thus a group of test particles at the same temperature as the bath would, as their off-diagonal elements shrunk, have a higher temperature, per our calculation of the thermal wavelength. Thus a system in equilibrium would not stay that way, contradicting thermodynamics as well.

The demonstration of Tegmark [4] claims not to use this assumption and has been quoted as if it were correct. Unfortunately it is not, and it violates energy conservation. The claim is made in [4]’s “Assumption 1” which is not about energy, only momentum. The breakdown in energy conservation comes from [4]’s “Assumption 2” which posits that a_{pk} , which, aside from a δ -function, is the T -matrix, is independent of p . With this assumption a (bath) particle striking a low energy (test) particle or a high energy (test) particle do the same thing. Another way to see this is by the thermodynamic argument used earlier: in a gas of two masses particles would scatter off one another, shortening off-diagonal matrix elements until they were smaller than the thermal wavelength, spontaneously heating the gas.

³ “No recoil” means that the particle struck does not move, although—and this is the point of Ref. [2]—its density matrix can change. For large mass objects this is reasonable, but breaks down for objects small enough for Brownian motion to be significant, surely at the level of 10^{-15} kg. (The latter is based on [9]. A water molecule has a mass of about 3×10^{-26} kg).

3.1 Kinematics

3.1.1 Kinematics of Collisions

Consider the collision of a test particle of mass M with a bath particle of mass m . The collision is elastic. Define the following momenta⁴:

Notation	Description	
\mathbf{p}	laboratory momentum of particle of mass M	
\mathbf{k}	laboratory momentum of particle of mass m	(3)
\mathbf{P}_{cm}	center of mass momentum	
$\boldsymbol{\varpi}$	relative momentum	

so that

$$\mathbf{P}_{\text{cm}} = \mathbf{p} + \mathbf{k}, \quad \boldsymbol{\varpi} = \frac{m\mathbf{p} - M\mathbf{k}}{m + M} \tag{4}$$

and

$$\mathbf{p} = \frac{M\mathbf{P}_{\text{cm}}}{m + M} + \boldsymbol{\varpi}, \quad \mathbf{k} = \frac{m\mathbf{P}_{\text{cm}}}{m + M} - \boldsymbol{\varpi}. \tag{5}$$

Moreover

$$d\mathbf{p}d\mathbf{k} = d\mathbf{P}_{\text{cm}}d\boldsymbol{\varpi}. \tag{6}$$

Quantities prior to the collision carry the subscript 0, post collision, 1. Thus

$$\mathbf{P}_{\text{cm},1} = \mathbf{P}_{\text{cm},0}, \quad |\boldsymbol{\varpi}_1| = |\boldsymbol{\varpi}_0| \tag{7}$$

(thereby inducing an implicit δ -function in integrals over $\boldsymbol{\varpi}_1$ and $\boldsymbol{\varpi}'_1$, where the prime is usually used for the second argument of ρ). Let $\psi(\mathbf{r})$ be the position representation wave function of the mass- M particle and $\widehat{\psi}(\mathbf{p})$ its momentum representation wave function. Taking $\hbar = 1$, we have $\psi(\mathbf{r}) = \int \widehat{\psi}(\mathbf{p}) \exp(i\mathbf{pr})d\mathbf{p}/(2\pi)^{3/2}$, with similar relations for $\widehat{\psi}$, $|\psi\rangle$, $|\mathbf{r}\rangle$ and $|\mathbf{p}\rangle$ (we write \mathbf{pr} for the inner product of the vectors).

It will be assumed that the collision is instantaneous, meaning short on a time scale in which other time evolution takes place. Our full quantum treatment ensures that the conservation laws for momentum and energy are valid (see Eq. (7)).

3.1.2 The Partial Trace

The reduced final density matrix, ρ_1 , of the mass- M test particle is obtained by tracing $|\Psi_1\rangle\langle\Psi_1|$ over the coordinates of the bath particle,

$$\rho_1 = \int d\mathbf{k}_1 \langle \mathbf{k}_1 | \Psi_1 \rangle \langle \Psi_1 | \mathbf{k}_1 \rangle, \tag{8}$$

where the scalar product is partial, to wit, *only* over the test particle degrees of freedom.

⁴ The symbol $\boldsymbol{\varpi}$ is not common in the physics literature and is a variant form of lower case pi. It is not omega-bar.

3.1.3 The S-Matrix

In the center of mass-system we write the elements of the S -matrix as $a(\varpi_1|\varpi_0)$, which because of unitarity satisfy

$$\int d\varpi_0 a(\varpi_1|\varpi_0)a^*(\varpi'_1|\varpi_0) = \delta(\varpi_1 - \varpi'_1). \tag{9}$$

3.1.4 The Reduced Density Matrix

When all the above material is used, the final result is an expression for the reduced density matrix, namely

$$\begin{aligned} \rho_1 &= \left(\frac{m+M}{M}\right)^6 \int d\mathbf{p}_1 d\mathbf{p}'_1 \int d\varpi_0 d\varpi'_0 \int d\varpi_1 a(\varpi_1|\varpi_0) \int d\varpi'_1 a^*(\varpi'_1|\varpi'_0) \\ &\times \rho_0^{\text{test}}(\mathbf{p}_1 - \varpi_1 + \varpi_0, \mathbf{p}'_1 - \varpi'_1 + \varpi'_0) \rho_0^{\text{bath}}\left(\frac{m}{M}(\mathbf{p}_1 - \varpi_1) - \varpi_0, \frac{m}{M}(\mathbf{p}'_1 - \varpi'_1) - \varpi'_0\right) \\ &\times \delta\left(\frac{m}{M}(\mathbf{p}_1 - \mathbf{p}'_1) - \frac{m+M}{M}(\varpi_1 - \varpi'_1)\right) |\mathbf{p}_1\rangle\langle\mathbf{p}'_1|. \end{aligned} \tag{10}$$

4 Collisions of Thermally Distributed Particles

4.1 Normalization of the Thermal State (Free Particle)

The thermal state of a free particle in empty space is not normalizable. As in Eq. (1), the cure is to put the particle in a box of volume V . Thus

$$\rho_{m,\beta}(\mathbf{p}, \mathbf{p}') = \frac{1}{Z_m} \langle \mathbf{p}' | e^{-\beta H} | \mathbf{p} \rangle = \frac{1}{Z_m} \delta_K(\mathbf{p}' - \mathbf{p}) e^{-\beta \mathbf{p}^2/2m}. \tag{11}$$

where δ_K is the Kronecker symbol, used for discrete momenta. Here, taking $V = L^3$, one writes

$$Z_m = \sum_{n=(n_x, n_y, n_z)} \exp\left(-\beta \frac{n^2 \pi^2}{2mL^2}\right) \equiv Vz_m, \tag{12}$$

where $Z_m \equiv Vz_m$ is a normalization factor and z_m is independent of V (and contains only β, m and constants). Similarly we define Z_M and z_M .

4.2 Reduced Density Matrix After Collision

We now show that if one starts with particles in equilibrium at inverse temperature β , it stays that way. With this assumption both bath and test particles have the corresponding initial density matrices. For the initial states this is assumed, but for the final density matrix of the test particle we must calculate.

Combining Eq. (10) with the state definitions given earlier we arrive at an expression for the reduced density matrix, *following* a collision. (Note that henceforth ρ_1 by itself is the reduced density matrix of the test particle alone.)

$$\begin{aligned}
 \rho_1(\mathbf{p}_1, \mathbf{p}'_1) &= \left(\frac{m+M}{M}\right)^6 \frac{1}{V^2} \frac{1}{z_m} \frac{1}{z_M} \int d\boldsymbol{\omega}_0 d\boldsymbol{\omega}'_0 d\boldsymbol{\omega}_1 d\boldsymbol{\omega}'_1 \\
 &\times a(\boldsymbol{\omega}_1|\boldsymbol{\omega}_0) a^*(\boldsymbol{\omega}'_1|\boldsymbol{\omega}'_0) \delta\left(\frac{m}{M}(\mathbf{p}_1 - \mathbf{p}'_1) - \frac{m+M}{M}(\boldsymbol{\omega}_1 - \boldsymbol{\omega}'_1)\right) \\
 &\times \delta(\mathbf{p}_1 - \boldsymbol{\omega}_1 + \boldsymbol{\omega}_0 - (\mathbf{p}'_1 - \boldsymbol{\omega}'_1 + \boldsymbol{\omega}'_0)) \\
 &\times \delta\left(\frac{m}{M}(\mathbf{p}_1 - \boldsymbol{\omega}_1 - \mathbf{p}'_1 + \boldsymbol{\omega}'_1) - \boldsymbol{\omega}_0 + \boldsymbol{\omega}'_0\right) \\
 &\times \exp\left(-\frac{\beta}{2M}|\mathbf{p}_1 - \boldsymbol{\omega}_1 + \boldsymbol{\omega}_0|^2\right) \exp\left(-\frac{\beta}{2m}\left|\frac{m}{M}(\mathbf{p}_1 - \boldsymbol{\omega}_1) - \boldsymbol{\omega}_0\right|^2\right).
 \end{aligned} \tag{13}$$

The δ -functions imply that

$$\boldsymbol{\omega}_1 - \boldsymbol{\omega}'_1 = \frac{m}{m+M}(\mathbf{p}_1 - \mathbf{p}'_1) \tag{14}$$

$$\mathbf{p}_1 - \mathbf{p}'_1 - (\boldsymbol{\omega}_1 + \boldsymbol{\omega}'_1) + \boldsymbol{\omega}_0 - \boldsymbol{\omega}'_0 = 0 \tag{15}$$

$$\frac{m}{M}(\mathbf{p}_1 - \mathbf{p}'_1 - (\boldsymbol{\omega}_1 - \boldsymbol{\omega}'_1)) + \boldsymbol{\omega}'_0 - \boldsymbol{\omega}_0 = 0. \tag{16}$$

It follows that $\boldsymbol{\omega}_0 = \boldsymbol{\omega}'_0$, $\mathbf{p}_1 = \mathbf{p}'_1$ and $\boldsymbol{\omega}_1 = \boldsymbol{\omega}'_1$. The product of the three δ -functions is therefore equivalent to

$$\left(\frac{m}{m+M}\right)^3 \delta(\mathbf{p}_1 - \mathbf{p}'_1) \delta(\boldsymbol{\omega}'_0 - \boldsymbol{\omega}_0) \delta(\boldsymbol{\omega}'_1 - \boldsymbol{\omega}_1). \tag{17}$$

The combined exponent in the Gaussian expressions in Eq. (13) is

$$\begin{aligned}
 &-\frac{\beta}{2} \left(\frac{|\mathbf{p}_1 - \boldsymbol{\omega}_1 + \boldsymbol{\omega}_0|^2}{M} + \frac{1}{m} \left| \frac{m}{M}(\mathbf{p}_1 - \boldsymbol{\omega}_1) - \boldsymbol{\omega}_0 \right|^2 \right) \\
 &= -\frac{\beta}{2} \left(\frac{m+M}{M^2} |\mathbf{p}_1 - \boldsymbol{\omega}_1|^2 + \frac{m+M}{mM} |\boldsymbol{\omega}_1|^2 \right) \\
 &= -\frac{\beta |\mathbf{p}_1|^2}{2M} - \frac{\beta \left| \boldsymbol{\omega}_1 - \mathbf{p}_1 \frac{m}{M+m} \right|^2}{2m} \left(\frac{M+m}{M} \right)^2,
 \end{aligned} \tag{18}$$

using $|\boldsymbol{\omega}_1| = |\boldsymbol{\omega}_0|$ (see Eq. (7)). Note that the exponentials are independent of $\boldsymbol{\omega}_0$ so that one can perform this integral in Eq. (13). Because of unitarity (Eq. (9)), Eq. (13) now has the square of $\delta(\boldsymbol{\omega}_1 - \boldsymbol{\omega}'_1)$ (the other δ -function comes from Eq. (17)). In Appendix A we deal with this issue by working with a finite box and using the Kronecker delta, for which there is no problem. Here we summarize those results.

Recall that in principle we are in a (large but) finite box of volume $V = L^3$, so that momenta are discrete and finely separated. The normalized wave functions are $\exp(i\boldsymbol{\omega}_0\mathbf{r})/\sqrt{V}$ and the action of the S -matrix is

$$S \frac{e^{i\boldsymbol{\omega}_0\mathbf{r}}}{\sqrt{V}} = \sum_{\boldsymbol{\omega}_1} a(\boldsymbol{\omega}_1|\boldsymbol{\omega}_0) \frac{e^{i\boldsymbol{\omega}_1\mathbf{r}}}{\sqrt{V}}. \tag{19}$$

Unitarity implies

$$1 = \left(S \frac{e^{i\boldsymbol{\omega}_0\mathbf{r}}}{\sqrt{V}} \middle| S \frac{e^{i\boldsymbol{\omega}'_0\mathbf{r}}}{\sqrt{V}} \right) = \frac{1}{V} \int_V d\mathbf{r} \sum_{\boldsymbol{\omega}_1, \boldsymbol{\omega}'_1} a(\boldsymbol{\omega}_1|\boldsymbol{\omega}_0) a^*(\boldsymbol{\omega}'_1|\boldsymbol{\omega}_0) e^{i(\boldsymbol{\omega}_1 - \boldsymbol{\omega}'_1)\mathbf{r}} \tag{20}$$

and

$$0 = \left(S \frac{e^{i\varpi'_0 r}}{\sqrt{V}} \middle| S \frac{e^{i\varpi_0 r}}{\sqrt{V}} \right) = \frac{1}{V} \int_V dr \sum_{\varpi_1, \varpi'_1} a(\varpi_1 | \varpi_0) a^*(\varpi'_1 | \varpi'_0) e^{i(\varpi_1 - \varpi'_1)r}. \tag{21}$$

The integral $\int_V dr/V$ gives $\delta_K(\varpi_1 - \varpi'_1)$, where the “ K ” indicates a *Kronecker* delta (taking values 0 and 1). Thus

$$\sum_{\varpi_1} a(\varpi_1 | \varpi'_0) a^*(\varpi_1 | \varpi_0) = \begin{cases} 1 & \text{if } \varpi'_0 = \varpi_0 \\ 0 & \text{if } \varpi'_0 \neq \varpi_0. \end{cases} \tag{22}$$

The foregoing is equivalent to taking, in the integral (9), “ dr ” = $\frac{\Delta n}{V} = \frac{1}{V}$.

Assembling all our results, we obtain

$$\begin{aligned} \rho_1(\mathbf{p}_1, \mathbf{p}'_1) &= \left(\frac{m+M}{M} \right)^3 \frac{1}{V} \frac{1}{z_m} \frac{1}{z_M} \delta(\mathbf{p}_1 - \mathbf{p}'_1) \exp\left(-\frac{\beta |\mathbf{p}_1|^2}{2M}\right) \\ &\times \int d\varpi_1 \exp\left(-\frac{\beta}{2m} \left(\frac{M+m}{M}\right)^2 \left| \varpi_1 - \frac{m\mathbf{p}_1}{M+m} \right|^2\right) \\ &= \frac{1}{V z_M} \delta(\mathbf{p}_1 - \mathbf{p}'_1) \exp\left(-\frac{\beta |\mathbf{p}_1|^2}{2M}\right) \equiv \rho_{M,\beta}(\mathbf{p}_1, \mathbf{p}'_1). \end{aligned} \tag{23}$$

We have thus shown that when particles in thermal states having the same β collide they remain in the thermal state. This has been demonstrated at the level of the density matrix. It follows that the notion that the off-diagonal elements in coordinate space decrease indefinitely is untenable.

4.3 Convergence to ρ_{th} with Many Collisions

In the previous subsection we have shown that the thermal state is a fixed point of the scattering process. Now we show that (subject to the assumption below) it is an attractor.

It would be natural to assume that the bath particles are already at equilibrium, but we will be more general and only assume the initial density matrix of the bath particle to be diagonal in p -space. Thus we take

$$\text{Bath density matrix} = \rho_{m,\beta}(\mathbf{p}, \mathbf{p}') = \delta(\mathbf{p} - \mathbf{p}') g_0(\mathbf{p})/V. \tag{24}$$

Suppose that after n independent collisions with bath particles the test particle has reduced density matrix $\rho_n(\mathbf{p} + \mathbf{q}/2, \mathbf{p} - \mathbf{q}/2)$. From Eq. (10) one obtains (note the slight change in notation for the arguments of the density matrix)

$$\begin{aligned} \rho_{n+1}(\mathbf{p} + \mathbf{q}/2, \mathbf{p} - \mathbf{q}/2) &= \frac{1}{V} \left(\frac{m+M}{M} \right)^3 \int d\varpi_0 d\varpi_1 a(\varpi_1 | \varpi_0) a^*(\varpi'_1 | \varpi'_0) \\ &\times \rho_n(\mathbf{p} + \mathbf{q}/2 - \varpi_1 + \varpi_0, \mathbf{p} - \mathbf{q}/2 - \varpi_1 + \varpi_0) \\ &\times g_0\left(\frac{m}{M} \left(\mathbf{p} + \frac{\mathbf{q}}{2} - \varpi_1\right) - \varpi_0\right). \end{aligned} \tag{25}$$

with $\varpi'_k = \varpi_k - m\mathbf{q}/(m+M)$. Between collisions ρ picks up a phase factor $\exp(-i\mathbf{p}\mathbf{q}t/m)$ (where t is the time between collisions) which does not affect the magnitude of the off-diagonal term and will not be noted further.

Equation (25) implies that the values of $\rho_{n+1}(\mathbf{p} + \mathbf{q}/2, \mathbf{p} - \mathbf{q}/2)$ depend only on ρ_n with the same \mathbf{q} value. In particular, the diagonal elements of ρ_{n+1} depend only on the diagonal elements of ρ_n . This has two consequences:

(1) Integrating Eq. (25) over \mathbf{p} yields

$$\int d\mathbf{p} |\rho_{n+1}(\mathbf{p} + \mathbf{q}/2, \mathbf{p} - \mathbf{q}/2)| \leq \int d\mathbf{p} |\rho_n(\mathbf{p} + \mathbf{q}/2, \mathbf{p} - \mathbf{q}/2)| C(\mathbf{p}, \mathbf{q}), \tag{26}$$

with

$$C(\mathbf{p}, \mathbf{q}) = \frac{1}{V} \left(\frac{m + M}{M} \right)^3 \left| \int d\boldsymbol{\omega}_0 d\boldsymbol{\omega}_1 a(\boldsymbol{\omega}_1 | \boldsymbol{\omega}_0) a^*(\boldsymbol{\omega}'_1 | \boldsymbol{\omega}'_0) \right. \\ \left. \times g_0 \left(\frac{m}{M} \left(\mathbf{p} + \frac{\mathbf{q}}{2} \right) - \frac{m + M}{M} \boldsymbol{\omega}_0 \right) \right| \begin{cases} = 1 & \text{if } \mathbf{q} = 0 \\ < 1 \text{ (strictly)} & \text{if } \mathbf{q} \neq 0. \end{cases} \tag{27}$$

To establish Eq. (27) use the Cauchy-Schwarz inequality for the a 's (which integrate to 1) and Eq. (22).

From Eq. (26) we deduce that in momentum space the non-diagonal elements of ρ_n go to zero.

(2) We next focus on the diagonal terms $\rho_n(\mathbf{p}, \mathbf{p})$. For each collision with a bath particle the probability distribution function $\rho_n(\mathbf{p}, \mathbf{p})$ becomes the function $\rho_{n+1}(\mathbf{p}, \mathbf{p})$ so that Eq. (25) is a master equation for a Markov chain in momentum space.

We next prove this assertion. Returning to Sec. 3.1, the momentum \mathbf{p} is the momentum of the M -particle after collision, and $\mathbf{p} - \boldsymbol{\omega}_1 + \boldsymbol{\omega}_0$ is its momentum before collision, the latter being the argument of ρ_n in Eq. (25). Moreover, the argument of g_0 in that equation (for $\mathbf{q} = 0$) is $\frac{m}{M}(\mathbf{p} - \boldsymbol{\omega}_1) - \boldsymbol{\omega}_0$ and is the momentum of the bath particle before collision (called \mathbf{k} in Sec. 3.1). Thus from Eq. (25) after the n^{th} collision the next momentum is

$$\mathbf{p}_{n+1} = \mathbf{p}_n + \delta\mathbf{p}, \quad \text{with } \delta\mathbf{p} = \boldsymbol{\omega}_1 - \boldsymbol{\omega}_0 = (\mathbf{R}_n - \mathbf{1}) \left(\frac{m\mathbf{p}_n - M\mathbf{k}_n}{M + m} \right), \tag{28}$$

where \mathbf{R}_n is a rotation in 3-space, $\mathbf{1}$ is the identity and \mathbf{k}_n is the momentum of the bath particle. The rotations, \mathbf{R}_n , are distributed according to $|a(\mathbf{R}_n \boldsymbol{\omega}_0 | \boldsymbol{\omega}_0)|$, which yields the probability distribution for $\delta\mathbf{p}$.

As a consequence the sequence \mathbf{p}_n represents the successive steps of a Markov chain in the momentum space of the M -particle. If this Markov chain is irreducible, its stationary distribution, if it exists, is unique and $\rho_n(\mathbf{p}, \mathbf{p})$ converges to the stationary distribution. In the case where g_0 is the thermal state of the bath particle we proved that Eq. (25) has a fixed point which is the thermal distribution of M -particle. As a consequence the density matrix ρ_n converges to the thermal state $\rho_{M,\beta}$. As to irreducibility (assumed earlier), this is equivalent to the assumption that the rotations \mathbf{R} are not the identity, which is guaranteed by the scattering not being trivial. ($g_0(\mathbf{p})$ is also assumed to be positive for all \mathbf{p} .)

5 Conclusions

Understanding the emergence of the classical world from the quantum has been a subject of interest—and contention. The concept of decoherence has been widely claimed to explain this phenomenon and to a large extent this conclusion has been based on calculations that demonstrate that the density matrix becomes effectively diagonal in coordinate space. As recognized in [2,3], this is not quite true. In particular, the $t \rightarrow \infty$ limit of the off-diagonal

configuration space density matrix does *not* vanish. In fact, these matrix elements do not become smaller than the thermal wavelength ($\lambda_{\text{th}} = \hbar/\sqrt{2\pi/mk_B T}$). Now λ_{th} can be quite small (of the order of angstroms for a gas at room temperature and pressure) but it is not zero.

What is interesting is that this is sufficient. To the extent that decoherence establishes that there are “definite” positions for the particles, the smallness of λ_{th} already provides for the desired degree of localization. There is no need to have ρ purely diagonal in coordinate space.

In this article we have shown that the thermal state is indeed preserved under scattering, and moreover, with technical assumptions, is in fact an attractor: a gas with internal scattering will tend toward the thermal state. The delicacy of our demonstrations suggests that sharper bounds on the convergence would depend on details of the scattering.

A traditional derivation of the Boltzmann factor for the thermal state starts with a system and reservoir, assuming that they pass only energy and that the reservoir’s temperature is not affected by the small amount of energy it gives to or takes from the system. One then assigns a probability to each particular state of the system proportional to the multiplicity of states in the reservoir, *given the energy of the system state*. Then, with a certain amount of hand-waving (including assumptions about additivity of entropy), one arrives at the thermal state. What does this have to do with scattering?

The short answer is we don’t know. It is likely that our assuming that the gas of scattering particles (of mass m) is already in the thermal state prejudices the final result. Whether the derivation *only* works with that assumption, or whether the final state of the mass- M particle (the test particle) follows that of the gas, is something that is beyond the scope of this paper.⁵

Finally, in Appendix B we provide a heuristic discussion of an alternative view of the entire scattering process. It reflects the perspective that a gas consists of a large number of particles that occasionally scatter off one another and is characterized by quantities such as the mean free path, ℓ . (All this is inherent in our previous work, but is not explicit.) The result of that Appendix is that if one were to treat the atoms as Gaussians (or coherent states)—a natural assumption—then the spread of those wave functions is *not* simply λ_{th} as one might have guessed, but is

$$\delta = \text{const} \sqrt{\ell \lambda_{\text{th}}}, \quad (29)$$

where δ is the wave packet spread and the constant is order unity. We present this Appendix as a further attempt to unify classical and quantum views, but, as indicated, the relation is not rigorous.

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Appendix A: Appendix to Sect. 4.2.

The calculations of Sec. 4.2 are delicate because formally they lead to squares of delta functions. To define them precisely we consider the case of a finite volume $V (= L^3)$ and

⁵ We do know that having the density matrix of the gas be diagonal in momentum space (but not necessarily in the thermal state) is enough to give the same property to that of the test particle. See Sect. 4.3.

make use of discrete momenta.

$$p = \frac{n\pi}{\sqrt{2/3}}, \quad n = (n_x, n_y, n_z). \tag{A1}$$

In this situation, Eq. (13) should be replaced by its discretized version, namely

1. replace the integrals over momenta by discrete sums,
2. replace $a(\mathbf{w}_1|\mathbf{w}_0)$ by $\tilde{a}(\mathbf{w}_1|\mathbf{w}_0) \equiv \frac{1}{V}a(\mathbf{w}_1|\mathbf{w}_0)$ with

$$S \frac{1}{\sqrt{V}} e^{i\mathbf{w}_0 r} = \sum_{\mathbf{w}_1} \tilde{a}(\mathbf{w}_1|\mathbf{w}_0) \frac{1}{\sqrt{V}} e^{i\mathbf{w}_1 r}, \tag{A2}$$

3. replace ρ by $\tilde{\rho} = \frac{1}{V}\rho$, and
4. replace g_0 by $\frac{1}{V}\tilde{g}_0$.

By the unitarity of the S matrix we then have

$$\sum_{\mathbf{w}_1} \tilde{a}(\mathbf{w}_1|\mathbf{w}'_0) \tilde{a}^*(\mathbf{w}_1|\mathbf{w}_0) = \delta_K(\mathbf{w}_0 - \mathbf{w}'_0), \tag{A3}$$

where δ_K is the Kronecker symbol. Eq. (A3) gives

$$\frac{1}{V} \sum_{\mathbf{w}_1} a(\mathbf{w}_1|\mathbf{w}'_0) a^*(\mathbf{w}_1|\mathbf{w}_0) = \delta(\mathbf{w}_0 - \mathbf{w}'_0), \tag{A4}$$

or

$$\int d\mathbf{w}_1 a(\mathbf{w}_1|\mathbf{w}'_0) a^*(\mathbf{w}_1|\mathbf{w}_0) = \delta(\mathbf{w}_0 - \mathbf{w}'_0). \tag{A5}$$

Moreover, in the continuum limit for \mathbf{w}_0 and \mathbf{w}'_0

$$V \delta_K(\mathbf{w}_0 - \mathbf{w}'_0) = \delta(\mathbf{w}_0 - \mathbf{w}'_0), \tag{A6}$$

and formally

$$\delta(0) = V. \tag{A7}$$

With this relation, Eq. (24) acquires meaning.

We return to Eq. (13) where $a \rightarrow \tilde{a}$ and the integrals over momenta are replaced by discrete sums. Then all delta functions are replaced by Kronecker symbols in Eqs. (17) and (13), so that

$$\begin{aligned} \tilde{\rho}_1(\mathbf{p}_1, \mathbf{p}'_1) &= \left(\frac{m+M}{M}\right)^3 \frac{1}{V^2 z_m z_M} \sum_{\mathbf{w}_0 \mathbf{w}'_0 \mathbf{w}_1 \mathbf{w}'_1} \tilde{a}(\mathbf{w}_1|\mathbf{w}_0) \tilde{a}^*(\mathbf{w}'_1|\mathbf{w}'_0) \\ &\quad \times \delta_K(\mathbf{p}_1 - \mathbf{p}'_1) \delta_K(\mathbf{w}'_0 - \mathbf{w}_0) \delta_K(\mathbf{w}'_1 - \mathbf{w}_1) \\ &\quad \times \exp\left(-\frac{\beta}{2M} |\mathbf{p}_1|^2\right) \exp\left(-\frac{\beta}{2m} \left(\frac{M+m}{M}\right)^2 \left|\mathbf{w}_1 - \mathbf{p}_1 \frac{m}{M+m}\right|^2\right), \end{aligned} \tag{A8}$$

where we have used Eq. (18). In Eq. (A8) the sum over ϖ_0 and ϖ'_0 reduces to $\delta_K(\varpi_1 - \varpi'_1)$ and the square of δ_K poses no problem. Therefore

$$\begin{aligned} \tilde{\rho}_1(\mathbf{p}_1, \mathbf{p}'_1) &= \left(\frac{m+M}{M}\right)^3 \frac{1}{V} \frac{1}{z_m} \frac{1}{z_M} \delta_K(\mathbf{p}_1 - \mathbf{p}'_1) \exp\left(-\frac{\beta}{2M} |\mathbf{p}_1|^2\right) \\ &\times \frac{1}{V} \sum_{\varpi_1} \exp\left(-\frac{\beta}{2m} \left(\frac{M+m}{M}\right)^2 \left|\varpi_1 - \mathbf{p}_1 \frac{m}{M+m}\right|^2\right). \end{aligned} \tag{A9}$$

This reduces to

$$\rho_1(\mathbf{p}_1, \mathbf{p}'_1) = \frac{1}{z_M} \delta(\mathbf{p}_1 - \mathbf{p}'_1) \exp(-\beta |\mathbf{p}_1|^2 / 2M), \tag{A10}$$

as desired and making use of Eq. (A7) to interpret $\delta(0)$.

As an example,

$$\begin{aligned} \tilde{\rho}_{n+1}(\mathbf{p} + \mathbf{q}/2, \mathbf{p} - \mathbf{q}/2) &= \frac{1}{V} \left(\frac{m+M}{M}\right)^3 \sum_{\varpi_0, \varpi'_1} \tilde{a}(\varpi_1 | \varpi_0) \tilde{a}^*(\varpi'_1 | \varpi'_0) \\ &\times \tilde{\rho}_n(\mathbf{p} + \mathbf{q}/2 - \varpi_1 + \varpi_0, \mathbf{p} - \mathbf{q}/2 - \varpi_1 + \varpi_0) \\ &\times \tilde{\xi}_0\left(\frac{m}{M} \left(\mathbf{p} + \frac{\mathbf{q}}{2} - \varpi_1\right) - \varpi_0\right). \end{aligned} \tag{A11}$$

An apparently difficult calculation is the one that proves that $C(\mathbf{p}, \mathbf{0}) = 1$, because it leads formally to $\delta(0)$ in the continuous calculation. But the discrete calculation, starting from Eq. (A11), poses no problem.

Appendix B: Heuristic Discussion of a Particle View of Scattering

In this Appendix we abandon rigor and present a heuristic justification of the formula $\delta = \text{const} \sqrt{\ell \lambda_{\text{th}}}$, where δ is the wave packet spread, ℓ is the scattering length, and the constant is order unity. In the forthcoming discussion we usually take \hbar and m equal to 1, so that $\lambda_{\text{th}} \sim \sqrt{\beta}$.

Our discussion reflects the tension between classical and quantum viewpoints. Quantum mechanically the density matrix reflects one’s knowledge of the particle wave function, but it does not demand a particular wave function. Thus one can write

$$\rho(x, y) \sim \exp\left(-\frac{m(x-y)^2}{2\beta\hbar^2}\right) \sim \int dk \exp\left(-\frac{2\beta\hbar^2 k^2}{m} + ik(x-y)\right) \tag{B1}$$

$(x, y, k \in \mathbb{R}^3)$, in which case the density matrix could represent a superposition of plane waves. But this is in sharp contrast to the classical picture of little balls bouncing around and scattering off each other. In the latter picture one would expect the *semi*-classical picture to be little wave packets, also occasionally scattering off each other (we assume the temperature and pressure of the gas to be such that particle identity can be ignored). After all there *is* a concept of mean free path (ℓ) for particles in a gas, and there is a relation between that and the quantum scattering cross section (σ), namely,

$$\ell = \frac{1}{n\sigma}, \tag{B2}$$

with n the particle density, per unit volume. Let us therefore picture our (monatomic) gas as a bunch of Gaussian wave packets occasionally scattering off each other. One thus writes

the same density matrix as a superposition of such packets. The individual wave packets are thus of the form

$$\psi(x) \sim \exp\left(-\frac{(x-x_0)^2}{2\delta^2} + ikx\right). \tag{B3}$$

One might identify the particle spread— δ —with λ_{th} but this would neglect an effect that until now was not necessary to take into account. Specifically, between scatterings the packet spreads. Thus a *free* particle that has the wave function of Eq. (B3), after a time t becomes

$$\psi(x, t) \sim \exp\left(-\frac{(x-x_0-kt)^2}{2(\delta^2+it/2)} + ikx\right). \tag{B4}$$

We next assume that the scattering shrinks the spread in the wave function back to its original value, reflecting the assumption of equilibrium. (More complicated scenarios can be envisioned, but we’re being both rough and simple.) Thus

$$\delta^2 = \frac{1}{\alpha} \sqrt{\delta^4 + t^2/4}, \tag{B5}$$

for some factor α . It is implicit that we still have roughly a Gaussian, as derived—with assumptions—in [10]. Note too that α is not the “effective value” of C of Eq. (27). The quantity α depends on details of the scattering matrix, but should be of order unity, so that

$$\alpha = \frac{\sqrt{\delta^4 + t^2/4}}{\delta^2} = O(1). \tag{B6}$$

The time, t , is the interval between scatterings, namely ℓ/v where ℓ is the mean free path and v is a characteristic velocity. In a gas at temperature $1/\beta$ this velocity is $\sqrt{1/\beta}$ (we also take Boltzmann’s constant to be 1). Thus the velocity is essentially λ_{th} and (after a bit of algebra) we have

$$\alpha^2 - 1 = \ell^2 \lambda_{\text{th}}^2 / \delta^4, \tag{B7}$$

or up to constants of order unity

$$\delta = \sqrt{\lambda_{\text{th}} \ell}. \tag{B8}$$

Of course this discussion totally lacks rigor, but it does provide some way of recovering the usual picture one has of an interacting gas, plus an observation that the wave packet spread and the thermal wavelength are related by the mean free path for scattering.⁶

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⁶ Since Eq. (B8) is dimensionally correct, our setting of \hbar, k_B and m to 1 has had no consequences.

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