ENERGY AND MOMENTUM CONSERVATION FOR DIFFUSION
- A STOCHASTIC MECHANICS APPROXIMATION - PART I

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ABSTRACT. This paper models the classical diffusion of a main particle through a heatbath by means of a pre-limit microscopic representation of its drifted momentum and energy transfers at collision times. The collision point linear interpolated path can be approximated by the solution to the "inscribed" continuous stochastic differential equation using the same drift function. Employing results from stochastic mechanics it is then shown that the combined main particle/heatbath system does not exchange or radiate energy if the probability distribution for the position of the main particle is derived from Schrödinger’s equation. Furthermore it is shown that the main particle distance traveled between collisions and the mean inter-collision time must satisfy a type of Minkowski invariant. Hence if there is a correlation between the pre- and post-collision velocities of the main particle through a collision point then the mean distance traveled can be related to the mean inter-particle collision times via a Lorentz transformation. The last Section shows that this approach can be applied to all elastic main particle/heatbath particle collisions either via direct calculation involving modeling the collision scattering or by altering the properties of the heatbath.

INTRODUCTION

Ever since Einstein’s introduction of the molecular-kinetic theory of heat in 1905 the Brownian motion/Markovian formalism has been applied to a large variety of topics including classical particle diffusion and stochastic mechanics. The first subject is more the domain of statistical mechanics and focusses on thermodynamic properties, Goldstein [1], isothermal flows Garbaczewski [2], transport equations (e.g. Master equation, Boltzmann’s equation or Kramer’s equation) and Markov Chains, for instance Posilicano [3], van Kampen [4] or Gamba [5]. The second topic falls under the interpretation of quantum mechanics see for instance the recent review by Carlen [6] or Nelson [7]. For a historical view on the development of Brownian Motion consult Nelson [8]. The present paper represents a (larger) particle (the "main" particle) diffusing through a heatbath of smaller particles employing a "finite-energy" Markovian difference equation and investigates various energy conditions using results that have been developed in stochastic mechanics.

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The simplifying assumption for diffusion is that the frequent energy exchanges between the main and heatbath particles induce a continual acceleration and deceleration that make the motion of the main particle look macroscopically as if it has no memory of its previous whereabouts. Mathematically the Brownian motion process is the result of a limiting procedure involving an infinite amount of collisions exchanging an infinite amount of energy. The original derivation of the associated diffusion equation for the density distribution is due to Einstein [9]. As a result of the limiting process the resulting Markovian process is not differentiable and therefore no energy or momentum can be ascribed to the main particle. Brownian motion is very attractive because of its "random step" intuition and because of the tractability of the associated diffusion equation.

Many ways of associating momentum and energy with the motion of a diffusing particle have been suggested in the literature. A straightforward and transparent approach is to augment the position process for the diffusing particle with a momentum process and investigate the position process in the limit that the momentum becomes extremely large. Modeling both position and momentum Nelson [8] showed that the position of the main particle converges in probability to the solution of a stochastic differential equation if the associated momentum process contains an ever larger mean reversion (and variance). The more typical - and mathematical - construction of Brownian motion is based on successive probabilistic additions of orthogonal functions, see Rogers & Williams [10] or Karatzas & Shreve [11]. These constructions do not consider the underlying particle collision process or the implied energy exchange between the main particle and heatbath environment.

This paper uses a direct approach by creating a pre-limit microscopic representation of a main particle by modeling its momentum and energy transfers at collision times. The assumption is that the collisions occur at stopping times \( t_j, j \geq 0 \) with \( t_{j+1} - t_j = \tau_j, j \geq 0 \), so that the main particle will have corresponding positions \( x_j \) at these collision times. Here \( \beta \) denotes the drift term \( b^\tau(x_j, t_j) \) and a Gaussian random shock. Since the particle drift over the interval \([t_j, t_{j+1}], j \geq 0\) is a function of \( x_j, t_j, j \geq 0 \), the position process of the main particle \( x_j, j \geq 0 \), reduces to a discrete Markovian stochastic process. The crucial assumption in this paper is that the inter-collision times \( \tau_j, j \geq 0 \), can be represented by a second (or higher) order gamma distribution. The main reason for this assumption is that the energy and momentum of the main particle between collisions are then well defined and finite with probability one.

The set of collision points \( \{x_j = x(t_j, \beta) | j = 0, 1, ...\} \) does not prescribe the position of the main particle at an arbitrary time \( t \notin \{ t_j | j = 0, 1, ...\} \). A reasonable estimate for the position of particle at time \( t \) is to define \( x(t, \beta) \), \( t \geq 0 \), as the linear interpolation on the collision positions. So \( x(t, \beta) \), is linearly interpolated from \( x(t_j, \beta) \) and \( x(t_{j+1}, \beta) \) where \( t_j \leq t < t_{j+1} \) \( (t_0 = 0, \text{ the origin}) \). The expectation is that if the number of collisions increases the process \( x(t, \beta) \in \mathbb{R}^n \), approaches the continuous stochastic process \( x(t) \in \mathbb{R}^n \), \( t \geq 0 \), which satisfies an appropriate stochastic differential equation with drift \( b^\tau(x, t) \). This obviously depends on the properties of the drift function, the variance function in the stochastic shock and the existence of collision points. Section 1 introduces a set of conditions for which
the discrete process $x(t,\beta)$ converges a.e. to the strong solution of a stochastic differential equation.

By design, if the particle experiences a collision at time $t$ with $x(t,\beta) = x$ then the next collision will occur at time $t + \tau_2$ while the last collision of the main particle occurred at time $t - \tau_1$. Hence the main particle has a (forward) momentum (and energy) towards the next collision equal $v_2 = (x(t + \tau_2) - x) / \tau_2$. The forward momentum is a random variable depending only on the current position of the main particle due to the fact that the stochastic process $x(t_j), j \geq 0,$ is Markovian. Similarly, the main particle will have a backward (or incoming) momentum (and energy) from the last collision equal $v_1 = (x - x(t - \tau_1)) / \tau_1$ since $t - \tau_1$ is the collision time previous to $t$. The backward momentum is a random variable that will have to be conditioned on the fact that it is now known that $x(t) = x$. At least in principle, the distribution for $x(t - \tau_1)$ follows from the distribution of the main particle for $x(t)$ employing Bayes' theorem. The forward and backward time step perspective for continuous stochastic processes can be gleaned from the extensive work on stochastic processes by Nelson [7], Carlen [12], [13], Guerra [14], [15] and see the references in Carlen [6].

Now that pre- and post-collision momenta and energies are determined for the main particle the collision process and energy exchange can be investigated for the main and heatbath particle. Section 2 investigates the consequences of an elastic collision and introduces the canonical linear relationship between the pre- and post collision velocities of the main and heatbath particle. This linear relationship is parameterized by a random anti-symmetric matrix $Z$ (manufactured from a random unitary matrix $U$) which incorporates the random center of mass line and collision impact angle information. This matrix will be referred to as the collision scattering matrix and collision energy exchanges with $Z \equiv 0$ are referred to as 'simple' collisions. Notice that in one dimension all collisions are simple.

Section 2 shows that the combined kinetic energy $H_k$ of the main and heatbath particle for simple elastic collisions can be expressed in the form of a simple quadratic combination of the forward and backward momenta/velocities of the main particle. In one dimension this relationship is exact while in more than one dimension the total kinetic energy $H_k$ of the colliding system refers to the energy of the motion along the center of mass line of the collision. The remaining kinetic energy of the main and heatbath particles is embedded in motion perpendicular to the collision center of mass line and remains invariant under the collision. Section 2 only investigates the canonical case where $H_k = H_k(Z \equiv 0)$ while Section 4 shows that the case $H_k = H_k(Z), Z \neq 0,$ can be reduced to the simple collision case.

Using this result Section 2 then shows that if the total kinetic energy of the system is not conserved then either the main particle is radiating energy into the heatbath or the main particle is absorbing energy from its heatbath surroundings. Such an exchange is possible as the result of external forces in the form of a potential $\Phi_p$ but in that case the combined kinetic energy $H_k$ and $\Phi_p$ together must be a conserved quantity, i.e. its expected value over all paths and positions must be a constant in time. The main result of the paper is that the only probability density that renders the total energy $E[H_k + \Phi_p]$ time invariant is the squared modulus of the wave function obtained from Schrödinger's equation. Appropriate conditions and examples for the potential will presented in Sections 2 and 4. This is a purely classical representation and Planck's constant is now replaced by a constant.
depending on the variance of the underlying stochastic process $\sigma^2$ and the main particle/heatbath particle mass ratio $\gamma$. This Section also shows (using collision elasticity) that the backward and forward momenta for the heatbath particle are tightly correlated if the main particle follows a Markovian path.

The main particle/heatbath particle elastic collision representation also provides a similar quadratic expression showing that the forward and backward velocities of the main particle are directly related to the (forward and backward) velocities of the heatbath particle. This relationship will often be referred to as the "momentum" constraint. Section 3 will show that if the heatbath particles are in energetic equilibrium with the main particle then the drift of the main particle and the correlation between the forward and backward velocities of the colliding heatbath particles must depend on the average inter-collision time. The relationship between the mean inter-particle collision time and the particle energy can be expressed in the form of the geometric Minkowski invariant. A consequence is that the mean distance traveled for the main particle and its mean inter-particle collision time can then be related via a Lorentz transformation.

The last Section focuses on the non-simple elastic collisions and qualifies the main and heatbath particle total energy dependence on the anti-symmetric scattering matrix $Z = Z(U)$. The same conservation of total energy employed in Section 2 now produces an equation which also contains the dynamics of the $Z$ matrix. The conservation result is discussed and some examples presented but no full solution for this case can be derived. However, the final results in this Section show that the total energy conservation and "momentum" constraint can be reformulated in terms of a transformed heatbath with heatbath particles that have a higher kinetic energy and a different correlation structure. It is possible therefore to transform the scattering matrix $Z$ away by subsuming it into the heatbath. Conveniently then all the results of Section 2 and 3 become valid again for the transformed heatbath.

The work is organized as follows. Section 1 introduces the details of the main particle collision representation and shows that the collision point linear interpolate converges a.e. to the solution of a continuous stochastic differential equation. Section 2 employs the fact that the particle collisions are elastic to show that a non-radiation condition demands that the only acceptable probability density for the position of the main particle is derived from Schrödinger’s equation. Section 3 uses the "momentum" constraint to show that the mean inter-particle collision time and inter-particle distance traveled satisfy a geometric Minkowski invariant. The last Section shows that the results of Sections 2 and 3 can be extended to almost all types of elastic collisions. All proofs have been delegated to the Appendices to make the paper more readable.

The notation employed in this this paper uses $E[.]$ or $E[. | .]$ for expectation or conditional expectation respectively. Typically $E[.]$ indicates an expectation over all variables between the brackets including the random scattering matrix $Z$ present and the forward and backward velocities. also $b^\pm(x, t) : \mathbb{R}^n \times [0, \infty) \mapsto \mathbb{R}^n$ are referred to as the forward and backward instantaneous drifts of the main particle and $\sigma(x, t) : \mathbb{R}^n \times [0, \infty) \mapsto \mathbb{R}^n \times \mathbb{R}^n$ are the corresponding variance terms. Moreover $\tau$ refers to the inter-particle collision time, $\tau = E[\tau]$ and $\beta = 2/\tau$. Often the reference to the time $t$ implicitly assumes that this time point is a collision time for the main particle. Clearly for finite mean collision times a distinction must be made between the collision points $t \in \{t_j, j = 0, 1, \ldots\}$ and the remaining time
points but the paper does not always complete the analysis. The norm $\| \cdot \|$ indicates the usual distance norm in $\mathbb{R}^n$.

1. Diffusion and Energy

This Section introduces the details of the $x_j = x(t_j, \beta)$, $j = 0, 1, \ldots$, collision representation, the converged process $x(t), t \geq 0$, and the distribution for the inter-particle collision times $\tau_j, j \geq 0$. It is shown that $\lim_{\beta \to \infty} x(t, \beta)$ exists under certain smoothness conditions and this Section also investigates the correlation between the forward and backward main particle velocities. Some results from Nelson and Carlen will be quoted without proof.

Following the Introduction let the collision points for the main particle be $x(t_j) \in \mathbb{R}^n, j = 0, 1, \ldots$, at collision time $t \in \{t_j, j = 0, 1, \ldots\}$, and assume that the next collision will occur in $x(t + \tau_2)$ at stopping time $t + \tau_2$. The collision previous to time $t$ occurred at $t - \tau_1$ when the main particle was in position $x(t - \tau_1)$. The collisions must be assumed "real" in the sense that the main particle actually interchanges energy with a colliding heatbath particle. The inter-collision times are modeled as independent random variables distributed with a second order Gamma distribution so that $f_{\beta}(t) = \beta^2 t e^{-\beta t}, t \geq 0$. As a result the time to the next collision $\tau_2$ and the time since the previous collision $\tau_1$ has the following moments

$$E[\tau_2] = E[\tau_1] = \int_0^\infty \beta^2 e^{-\beta t} dt = \frac{2}{\beta} = \tau,$$

$$\text{var}(\tau_2) = \text{var}(\tau_1) = \frac{2}{\beta^2} = \frac{1}{2} \tau^2.$$  

Most importantly for this distribution it is also true that

$$E \left[ \frac{1}{\tau_2} \right] = \frac{E \left[ \tau_1 \right]}{E \left[ \tau_1 \right]} = \int_0^\infty \beta^2 e^{-\beta t} dt = \beta = \frac{2}{\tau},$$

$$E \left[ \frac{1}{\sqrt{\tau_2}} \right] = E \left[ \frac{1}{\sqrt{\tau_1}} \right] = \int_0^\infty \beta \sqrt{\beta} e^{-\beta t} dt = \sqrt{\frac{2\pi}{\beta}}.$$  

Higher order Gamma distributions could have been employed for the inter-collision times or in fact any distribution such that $E[\tau^{-1}] < \infty$ would have been suitable but there seems little fundamental difference in the analysis. Interestingly, the ubiquitous exponential distribution is excluded due to the last restriction but notice that the second order Gamma distribution is the distribution of the sum of two exponential random variables.

By assumption above if $t$ is a collision time with main particle position $x(t, \beta) = x \in \mathbb{R}^n$ then the previous collision occurred at $t - \tau_1$. In this case $\tau_1$ is a random variable conditional on the fact that a collision occurred in the future $t$ with the particle in position $x(t, \beta) = x \in \mathbb{R}^n$. Unfortunately, the distribution for $\tau_1$ conditional on this event is no longer a second order Gamma distribution, see Feller [16] for a more complete discussion. The future conditioning alters the distribution of $\tau_1$ which is easy to see since any collision time $t - \tau_1$ previous to $t$ must satisfy $0 \leq t - \tau_1 \leq t$. Hence $0 \leq \tau_1 \leq t$ counter to the domain definition of a Gamma distribution. Moreover, there is always the possibility that no previous collision occurred so the real density for $\tau_1$ is in fact defective. However, for $t \gg \tau$ it is reasonable to assume that $\tau_1$ is at least approximately a second order Gamma distribution with $E[\tau_1] = E[\tau_2]$ and $E[\tau_1^{-1}] = E[\tau_2^{-1}]$. 

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Theorem implies that ∆⁻backward drift used in stochastic mechanics and for sufficiently large $\tau_1$, $\tau_2$ are the inter-collision stopping times with (independent) second order Gamma distributions with $b^\pm(x, t) : \mathbb{R}^n \times [0, \infty) \mapsto \mathbb{R}^n$ and $\sigma(x, t) : \mathbb{R}^n \times [0, \infty) \mapsto \mathbb{R}^n \times \mathbb{R}^n$ as the drift vector and variance matrix respectively. Here $\beta = 2/\tau = E[\tau_2^{-1}] = E[\tau_1^{-1}]$, see equation (1.1), and $\Delta^\pm z = z(t_{j+1}) - z(t)$ where $z(t) \in \mathbb{R}^n, j \geq 0$, is a Gaussian process and $\Delta^- z$ is a Gaussian increment independent of $\Delta^+ z$ with $E[(\Delta^- z)_j^2] = \tau_1$.

Due to the aforementioned issue with the distribution for $\tau_1$ the postulated form for the backward velocity in (1.2b) cannot be correct. For fixed $\tau_2$ and $\tau_1$ Bayes’ Theorem implies that $\Delta^- x(t, \beta)$ must have a Gaussian distribution but not necessarily with the same variance matrix $\sigma = \sigma(x, t, \beta)$. As $\tau_1$ and $\tau_2$ are random variables the forward increment is no longer Gaussian and the distribution of the backward velocity distribution is unclear. Therefore equation (1.2b) should have been written as

$$x(t, \beta) - x(t - \tau_1, \beta) = \Delta^- x(t, \beta) = b^-_\beta(x(t, \beta), t)\tau_1 + \sigma\Delta^- z,$$

with

$$b^-_\beta(x(t, \beta), t) = \frac{E[\Delta^- x(t, \beta) | x(t, \beta)]}{\tau_1},$$

$$\sigma\Delta^- z = \Delta^- x(t, \beta) - b^-_\beta(x(t, \beta), t)\tau_1,$$

where again $E[\Delta^- z] = \tau_1$. Furthermore for finite $\beta$ the increment $\Delta^- z$ is not a Gaussian increment. However the expectation is that for progressively smaller average inter-particle collision times ($\tau \to 0$) that $b^-_\beta(x, t) \to b^-_\beta(x, t), \sigma_\beta \to \sigma$ and $\Delta^- z$ becomes approximately Gaussian. In other words $b^-_\beta(x, t)$ approaches the backward drift used in stochastic mechanics and for sufficiently large $\beta$ (small $\tau$) equation (1.2d) approaches (1.2b). Equation (1.2d) is therefore a definition while (1.2b) is only true in the limit of sufficiently small time steps.

Due to (1.2a), (1.2b) the forward and backward velocities can now be written as

$$v_2(x(t), t, \beta) = \frac{x(t + \tau_2, \beta) - x(t, \beta)}{\tau_2} = b^+(x(t), t) + 1 \frac{\sigma\Delta^+ z}{\tau_2},$$

$$v_1(x(t), t, \beta) = \frac{x(t, \beta) - x(t - \tau_1, \beta)}{\tau_1} = b^-(x(t), t) + 1 \frac{\sigma\Delta^- z}{\tau_1},$$

which is properly defined because the diffusion shocks $\sigma\Delta^+ z/\tau_2$ and $\sigma\Delta^- z/\tau_1$ are proper random variables with distribution $f_{\Delta^\pm z}(v) \sim \left(\beta + \frac{\alpha^2}{\tau}\right)^{-5/2}$. In fact it is straightforward to show that

$$E[v_2(x(t), t, \beta) | x(t)] = b^+(x(t), t),$$

$$E[v_1(x(t), t, \beta) | x(t)] = b^-_\beta(x(t), t),$$

$$Cov[v_1(x)] = Cov[v_2(x)] = \frac{4}{\tau}\sigma\sigma^T,$$
using the fact that $E\left[\tau_2^{-1}\right] = E\left[\tau_1^{-1}\right] = 2/\sigma$ from equation (1.1). The expectations and covariances were calculated conditional on the collision occurring at time $t$.

To define the solution to the difference equation properly, fix a time interval $[0, T]$ and consider the collision set in this time interval $x(t_j, \beta), j = 1, \ldots, N$, for a random variable $N$ such that $t_N \leq T$ and $t_{N+1} > T$. Hence $N$ is the last collision in the time interval $[0, T]$. Define $N(t) = \max_{j \in \{0, 1, \ldots\}} \{t_j | t_j < t\}$ with $t_{mn} = t_{N(t)}, t_{mx} = t_{N(t)+1}$ then

$$x(t, \beta) = \begin{cases} \alpha_1 x(t_{mn}, \beta) + (1 - \alpha_1)x(t_{mx}, \beta), & \text{if } N(t) \geq 0, \\ x(0), & \text{if } N(t) = \infty, \end{cases}$$

(1.4)

where $N = \infty$ is an event that has probability zero as the particle inter-collision times are all finite and identically distributed. Hence $P\left[N(t) < \infty\right] = 1$ so that $t_{mx}$ and $t_{mn}$ are well defined with probability 1. An alternative expression used by the Theorem below is the following martingale representation $x(t, \beta) = x_N + b(x_N, t_N)(t - t_N) + \sigma \Delta(t - t_N)$ which differs from (1.4) only by the proportionality on the Gaussian shock.

The point of the Theorem below is to show under what circumstances $x(t, \beta) \to x(t), a.e.$, where the position process $x(t)$ is a strong solution to the stochastic differential equation corresponding to (1.2a) with drift $b^+(x(t), t)$ and variance matrix $\sigma = \sigma(x(t), t)$.

**Theorem 1.1.** Let the forward drift terms $b^+(x, t) : \mathbb{R}^n \times [0, T] \to \mathbb{R}^n$ and variance matrix $\sigma(x, t) : \mathbb{R}^n \times [0, T] \to \mathbb{R}^n \times \mathbb{R}^n$ satisfy the following growth and global Lipschitz condition

$$\|b^+(x, s) - b^+(y, s)\| + \|\sigma(x, s) - \sigma(y, s)\| \leq K \|x - y\|,$$

$$\|b^+(x, s)\|^2 + \|\sigma(x, s)\|^2 \leq K^2 \left(1 + \|x\|^2\right),$$

(1.5)

for all $x, y \in \mathbb{R}^n$ and $s \in [0, T]$. Let the drift function also satisfy a Lipschitz condition in time such that a constant $M_f$ exists so that

$$\|b^+(x, s) - b^+(x, t)\| \leq M_f |s - t|,$$

(1.6)

for all $x \in \mathbb{R}^n$, and all $s, t \in [0, T]$. Let $x(t, \beta)$ be the position of the main particle at time $t$ due to a finite set of collisions as specified in (1.2a) and (1.3), i.e.

$$x(t, \beta) = x_0 + \sum_{j=0}^{j=N} v_2(x(t_j, \beta)) \tau_j,$$

(1.7)

$$= x_0 + \sum_{j=0}^{j=N} \left[ b^+(x(t_j, \beta), t_j) \tau_j + \sigma \Delta^+ z_j \right],$$

where $\tau_j = t_{j+1} - t_j, 0 \leq j < N(t), \tau_{N(t)} = t - t_{N(t)-1}, t_0 = 0, t_{N(t)+1} = t$ (not a collision point) and where $\Delta^+ z_j = z(t_{j+1}) - z(t_j), z(t) \in \mathbb{R}^n, j = 0, 1, \ldots, N(t)$ are the Gaussian pulses.

Let $x_0 = x(\beta, 0) = x(0)$ be a random variable such that $E[x_0^2] < \infty$ then $x(t, \beta) \to x(t)$ almost everywhere as $\beta \uparrow \infty$ for the process $x(t)$ satisfying the
stochastic differential equation
\[ x(t) = x_0 + \int_0^t b^+ (x(s), s) \, ds + \int_0^t \sigma dz(t). \] (1.8)

Remark 1.2. Condition (1.5) together with \( E[ x_0^2 ] < \infty \) ensure that there is a strong solution \( x(t), t \in \mathbb{R}, \) to equation (1.8). This means that \( x(t) \in \mathbb{R}^n \) is a continuous process adapted to the filtration \( \{ \mathcal{F}_t; 0 \leq t < \infty \} \) of the probability space \( (\Omega, \mathcal{G}, P) \) and that
\[
P \left[ \int_0^t \left[ |b^+ (x(s), s)| + \sigma_{ij}^2 (x(s), s) \right] \, ds < \infty \right] = 1, \tag{1.9} \]
for all \( i, j = 1, \ldots, n. \) Condition (1.6) is not required for a strong solution but is an essential condition for the convergence. The filtration \( \{ \mathcal{F}_t; 0 \leq t < \infty \} \) encompasses the \( \sigma \)-algebra of events associated with the initial condition \( x_0 \) (a random variable) and the \( \sigma \)-algebra associated with the stochastic process \( z(t), t \geq 0. \) The solution is unique (any two solutions are equal with probability one) and can be written as a functional of the initial condition and a realization of the Gaussian process \( z(t); 0 \leq t < \infty. \)

Remark 1.3. A strong solution for (1.8) implies a growth condition on the second moment of \( x(t), t > 0 \) such that
\[
E \left[ x(t)^2 \right] \leq C \left( 1 + E \left[ x_0^2 \right] \right) e^{Ct},
\]
for some appropriate constant \( C > 0. \) In the case of few interactions no collisions occur before \( t = t_N (\beta \downarrow 0) \) so then (1.7) reduces to
\[
x(t, 0) = x_0 + [b^+(x_0, 0)t + \sigma \Delta^+ z_0],
\]
with \( \Delta^+ z_0 = z(t) - z(0). \) Then
\[
E \left[ x(t, 0)^2 \right] = E \left[ x_0^2 \right] + E \left[ b^+(x_0, t_j)^2 t_j^2 + \sigma^2 t_j \right] \\
\leq E \left[ x_0^2 \right] + K^2 E \left[ x_0^2 \right] t_j^2 + \sigma^2 t < \infty,
\]
from the growth condition (1.5).

Proof. For the sake of convenience the variance matrix will be assumed to be constant which does not materially alter the proof. Fix \( N \) then
\[
\| x(t, \beta) - x(t) \| = \left\| \sum_{j=0}^N \int_{t_j}^{t_{j+1}} \left[ b^+ \left( x(t_j, \beta), t_j \right) - b^+ \left( x(s), s \right) \right] \, ds \right\| \tag{1.10}
\]
\[
\leq \sum_{j=0}^N \int_{t_j}^{t_{j+1}} \left\| b^+ \left( x(t_j, \beta), t_j \right) - b^+ \left( x(s), s \right) \right\| \, ds.
\]
Because of (1.5) and (1.6) the integrand can be majorized as
\[
\left\| b^+ \left( x(t_j, \beta), t_j \right) - b^+ \left( x(s), s \right) \right\| \\
\leq \left\| b^+ \left( x(t_j, \beta), t_j \right) - b^+ \left( x(s), t_j \right) + b^+ \left( x(s), t_j \right) - b^+ \left( x(s), s \right) \right\| \\
\leq \left\| b^+ \left( x(t_j, \beta), t_j \right) - b^+ \left( x(s), t_j \right) \right\| + \left\| b^+ \left( x(s), t_j \right) - b^+ \left( x(s), s \right) \right\| \\
\leq \left\| b^+ \left( x(t_j, \beta), t_j \right) - b^+ \left( x(s), t_j \right) \right\| + M_f |t_j - s|,
\]
and applying this to (1.10) results in
\[ \|x(t, \beta) - x(t)\| \]
\[ \leq \sum_{j=0}^{j=N} \int_{t_j}^{t_j+1} \|b^+ (x(t_j, \beta), t_j) - b^+ (x(s), t_j)\| \, ds \]
\[ + M_f \sum_{j=0}^{j=N} \int_{t_j}^{t_j+1} |t_j - s| \, ds \]
\[ \leq K \sum_{j=0}^{j=N} \sup_{t_j \leq s \leq t_{j+1}} \|x(t_j, \beta) - x(s)\| \tau_j + \frac{M_f}{2} \sum_{j=0}^{j=N} \tau_j^2. \]  
(1.11)

and so
\[ \sup_{t_N \leq s \leq t} \|x(t_N, \beta) - x(s)\| \]
\[ \leq K \sum_{j=0}^{j=N} \sup_{t_j \leq s \leq t_{j+1}} \|x(t_j, \beta) - x(s)\| \tau_j + \frac{M_f}{2} \sum_{j=0}^{j=N} \tau_j^2. \]

To extract the growth of the sup_{t_j \leq s \leq t_{j+1}} \|x(t_j, \beta) - x(t_j)\| term from this inequality the following discrete version of Gronwall’s Inequality will be applied, see Shreve [11].

**Lemma 1.4.** Let \( a_n > 0, n = 0, 1, \ldots \) be a set of numbers such that
\[ a_n \leq \sum_{j=0}^{j=n-1} (P_j a_j) + Q_n, \quad n = 1, \ldots, \]  
(1.12)

for positive numbers \( P_j, Q_j, j = 0, 1, \ldots \). Then for all \( n > 0 \)
\[ a_n \leq a_0 P_0 \prod_{j=0}^{j=n-1} + \left( Q_n + \sum_{k=1}^{k=n-1} \frac{\prod_{k}^{k=n-1}}{P_k} Q_k \right), \quad n = 1, \ldots, \]  
(1.13)

where \( \Pi_n = \prod_{j=0}^{j=n} (1 + P_j), n = 0, 1, \ldots \)

**Proof.** From (1.12) it follows that
\[ a_n = \sum_{j=0}^{j=n-1} P_j a_j + Q_n - z_n, \quad n = 1, \ldots, \]  
(1.14)

for some positive sequence of numbers \( z_n > 0, n = 1, \ldots \). Let \( \beta_n = \sum_{j=0}^{j=n} P_j a_j, n = 0, 1, \ldots \), then (1.14) can be written as
\[ \beta_n = (1 + P_n) \beta_{n-1} + P_n (Q_n - z_n), \quad n = 1, \ldots, \]

with initial condition \( \beta_0 = P_0 a_0 \). The solution to this equation equals
\[ \beta_n = \beta_0 \frac{\Pi_n}{\Pi_0} + \sum_{k=1}^{k=n} \frac{\Pi_n}{\Pi_k} P_k (Q_k - z_k), \]
using $\Pi_n = \prod_{j=0}^{j=n} (1 + P_j)$. Finally then

$$P_n a_n = \beta_n - \beta_{n-1}$$

$$= \beta_0 \left( \frac{\Pi_n - \Pi_{n-1}}{\Pi_0} \right) + P_n Q_n + (\Pi_n - \Pi_{n-1}) \sum_{k=1}^{k=n-1} \Pi_k^{-1} P_k Q_k$$

$$- P_n z_n - (\Pi_n - \Pi_{n-1}) \sum_{k=1}^{k=n-1} \Pi_k^{-1} P_k z_k$$

$$= \beta_0 P_n \frac{\Pi_{n-1}}{\Pi_0} + P_n \left( Q_n + \sum_{k=1}^{k=n-1} \frac{\Pi_{n-1}}{\Pi_k} P_k Q_k \right)$$

$$- P_n \left( z_n + \Pi_{n-1} \sum_{k=1}^{k=n-1} \Pi_k^{-1} P_k z_k \right),$$

since $\Pi_n - \Pi_{n-1} = \Pi_n - (1 + P_n) - \Pi_{n-1} = P_n \Pi_{n-1}$. Now $\beta_0 = P_0 a_0$ and $z_n \geq 0, n \geq 1$, so dividing by $P_n$ it follows that

$$a_n \leq a_0 P_n \frac{\Pi_{n-1}}{\Pi_0} + \left( Q_n + \sum_{k=1}^{k=n-1} \frac{\Pi_{n-1}}{\Pi_k} P_k Q_k \right). \tag{1.15}$$

If all $P_n, Q_n, n = 0, 1, \ldots$ are equal so that $P_n = P, Q_n = Q, n = 0, 1, \ldots$ then (1.15) reduces to

$$a_n \leq (P a_0 + Q)(1 + P)^{n-1}, \quad n = 1, \ldots, \tag{1.16}$$

Notice that the righthand side of (1.16) increases monotonically with $n$. \hfill $\square$

Applying (1.13) to (1.11) using $\Pi_n = \prod_{j=0}^{j=n} (1 + K \tau_j), P_n = K \tau_n, n \geq 0$ and $Q_n = \frac{M_f}{2} \sum_{j=0}^{j=n} \tau_j^2, n \geq 0$, with the last remark in the Lemma, it follows that

$$\sup_{t_N \leq s \leq t} \|x(t_N, \beta) - x(s)\| \leq \|x(0, \beta) - x(0)\| K \tau_0 \frac{\Pi_N}{\Pi_0} \tag{1.16}$$

$$+ \frac{M_f}{2} \left( \sum_{j=0}^{j=N} \tau_j^2 + \sum_{k=1}^{k=N} \frac{\Pi_N}{\Pi_k} K \tau_k \sum_{j=0}^{j=k-1} \tau_j^2 \right), \tag{1.17}$$

Now $x(0, \beta) = x(0)$ and also

$$\Pi_N = \prod_{j=0}^{j=N} (1 + K \tau_j) = e^{\sum_{j=0}^{j=N} \log(1 + K \tau_j)} \leq e^{K t},$$

hence (1.16) reduces to

$$\max_{0 \leq j \leq N} \sup_{t_j \leq s \leq t_{j+1}} \|x(s, \beta) - x(s)\|$$

$$\leq \frac{M_f}{2} \left( \sum_{j=0}^{j=N} \tau_j^2 \right) (1 + K T e^{K T}),$$

so that finally

$$E \left[ \sup_{0 \leq t \leq T} \|x(t, \beta) - x(t)\| \right] \leq \frac{L}{\beta},$$
where

\[ L = 3M_f T (1 + KT e^{KT}) \, . \]

This is the result of the fact that \( E \left( \sum_{j=0}^{N} \tau_j^2 \right) = 3T \mathfrak{T} \) and the fact that \( t_{N+1} = t \).

From Chebychev then

\[ Pr \left[ \sup_{0 \leq t \leq T} \left| x(t, 2^{2k}) - x(t) \right| \geq \frac{1}{2^k} \right] \leq \frac{L}{2^k}, \]

so that by Borel-Cantelli \( x(t, \beta) \longrightarrow x(t) \) almost everywhere on the interval \([0, T]\) if \( \mathfrak{T} \downarrow 0 \). This completes the proof. \( \Box \)

Remark 1.5. This result justifies posing equation (1.2a) to specify the discrete dynamics of the main particle and use the solution \( x(t), t \geq 0 \) (1.8) as an approximation of \( x(t, \beta), t \geq 0 \). Clearly the discrete subordinate process that solves (1.2a) is difficult to determine. The theorem above does not address the validity of equation (1.2b) nor does it provide a hint as to the form of the backward drift \( b^- (x, t) \).

Remark 1.6. Unfortunately, the types of solutions that are most of interest have drift terms \( b^+(x, t) \) that can be singular and therefore do not satisfy conditions (1.5) and (1.6). However, Carlen showed in [13] that for a wide array of interesting drift functions a weak solution exists for \( x(t), t \in \mathbb{R}^n \). Hence a filtration \( \{ F_t; 0 \leq t < \infty \} \) exists for which conditions (1.8) and (1.9) are satisfied. In this case uniqueness does not necessarily hold (in the same fashion) and no (measurable) functional exists to map the solution given the initial condition and the Brownian path. It is not clear at all how Theorem (1.1) can be generalized to appropriate weak solutions of equations (1.8) and (1.9). For more discussion on strong and weak solutions in the present context, see Shreve [11], Rogers [10], or Carlen [12].

Following Nelson [7] and Carlen [12] it can be shown that the backward increment for a continuous stochastic process is equivalent to a time reversed Markovian process with a related drift and Gaussian increment. Specifically the following applies.

**Theorem 1.7.** If conditions (1.5) and (1.6) apply, let \( \sigma \equiv \sigma I \) so that the variance matrix \( \sigma \) is constant. Then, for a diffusion process \( x(t) \in \mathbb{R}^n \) the forward motion of the particle \( x(t + \tau_2) - x(t) \) and the backward step \( x(t) - x(t - \tau_1) \) conditional on \( x(t) = x \) are given by

\[ x(t + \tau_2) - x(t) = \Delta^+ x(t) = b^+(x(t), t) \tau_2 + \sigma \Delta^+ z, \quad (1.18a) \]

\[ x(t) - x(t - \tau_1) = \Delta^- x(t) = b^- (x(t), t) \tau_1 + \sigma \Delta^- z, \quad (1.18b) \]

\[ b^- (x, t) = b^+ (x, t) - \sigma^2 \frac{\nabla \rho(x, t)}{\rho(x, t)}, \quad (1.18c) \]

where \( \rho(x, t) \in \mathbb{R}, x \in \mathbb{R}^n \) is the probability density for finding the main particle at position \( x \) at time \( t \). The shocks \( \Delta^+ z \) and \( \Delta^- z \) are independent Gaussian increments with mean zero and variances \( \tau_2 \) and \( \tau_1 \) respectively. From this it follows
that

\[ \rho(x,t) = -\nabla \left( b^+ (x,t) \rho(x,t) \right) + \Delta_x \rho(x,t), \]  
(1.19a)

\[ \rho(x,t) = -\nabla \left( b^- (x,t) \rho(x,t) \right) - \Delta_x \rho(x,t), \]  
(1.19b)

so that

\[ \rho(x,t) = -\nabla \left( \frac{b^+ (x,t) + b^- (x,t)}{2} \right) \rho(x,t), \]  
(1.19c)

which is the continuity equation. Here \( \nabla = \left( \frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n} \right) \), \( \Delta_x = \left( \frac{\partial^2}{\partial x_1^2}, \ldots, \frac{\partial^2}{\partial x_n^2} \right) \) and \( (\cdot) \) denotes the time derivative.

**Proof.** See references Nelson [2] and Carlen [12] and the references therein for proofs where the collision times are infinitesimally small. For the justification of (1.18a), (1.18b) and (1.18c) see remark (1.9) below.

**Remark 1.8.** From this point onward no distinction will be made between \( x(t,\beta) \) and \( x(t) \) as the latter can be obtained as the limit of the former. This is not only to relieve notation but also to emphasize the fact that the results that are to follow are only true in the limit of \( \beta \uparrow \infty \).

**Remark 1.9.** Equation (1.18a) is exact by definition and its solution approaches \( x(t), t \geq 0 \), which has a probability density \( \rho(x,t) \) and a forward drift \( b^+ (x,t) \). Therefore the backward drift \( b^- (x,t) \) can be obtained as a result of (1.18c). As a result equation (1.19c) is approximately correct for small discrete time steps.

The Corollary below uses Ito’s Lemma and (1.8) to find an approximation for a function of the position \( x(t) \).

**Corollary 1.10.** For any function

\[ \Delta^+ f = f(x(t+\tau_2),t+\tau_2) - f(x(t),t) \]
\[ = (f_t + \sigma^2 \Delta_x f)\tau_2 + \nabla f . \Delta^+ x(t) + O(\tau_2) \]
(1.20)

and

\[ \Delta^- f = f(x(t),t) - f(x(t-\tau_1),t-\tau_1) \]
\[ = (f_t - \sigma^2 \Delta_x f)\tau_1 + \nabla f . \Delta^- x(t) + O(\tau_1), \]
(1.21)

where \( \Delta^+ \), \( \Delta^- \), \( \tau_1 \) and \( \tau_2 \) are introduced in Theorem (1.17) above.

**Proof.** Equation (1.20) follows from Ito’s Lemma, while for (1.21) it is clear that

\[ f(x(t-\tau_1),t-\tau_1) = f(x(t) - \Delta^- x, t - \tau_1) \]
\[ = f(x(t),t) - f_t \tau_1 - f_x \Delta^- x + \frac{1}{2} f_{xx} (\Delta^- x)^2 + O(\tau_1), \]

so

\[ \Delta^- f = f(x(t),t) - f(x(t-\tau_1),t-\tau_1) \]
\[ = f_t \tau_1 + f_x \Delta^- x - \frac{1}{2} f_{xx} (\Delta^- x)^2 + O(\tau_1) \]
\[ = (f_t - \sigma^2 f_{xx}) \tau_1 + f_x \Delta^- x(t) + O(\tau_1), \]

which settles the proof. \( \square \)
Remark 1.11. Consider the one-dimensional case where \( x(t) \in \mathbb{R} \) and assume that the variance term depends on \( x(t) \) and \( t \) explicitly so that \( \sigma = \sigma(x(t), t) \). If the variance process is at least once differentiable then the backward and forward representation can still be obtained as follows. Let \( y = f(x, t) = \int_{-\infty}^{x} \frac{\sigma(p, t)}{\sigma(p, t)} dp \) and let \( \rho_f(y) \) be the density function for \( y \) at time \( t \) then using Ito’s formula

\[
\begin{align*}
\Delta^+ y &= F^+(y, t) dt + \sigma^+ \Delta z \\
 &= \left( f_t + b^+ \nabla f + \frac{\sigma^2}{2} \Delta x f \right) dt + \sigma_r \Delta^+ z, \\
\Delta^- y &= F^-(y, t) dt + \sigma_r \Delta^- z,
\end{align*}
\]

where

\[
F^-(y, t) = F^+(y, t) - \sigma^2 \frac{\partial f}{\partial y},
\]

and where \( \Delta^+ z \) and \( \Delta^- z \) are the increments as defined above. Inverting the function above \( x(y) = f^{-1}(y, t) \) and writing \( \frac{\partial \rho}{\partial x} = \rho_x \), the probability density for \( y \) can then be translated back.

Returning to the backward and forward representation of the motion of the main particle in (1.2a), (1.2a) the following is now straightforward.

**Lemma 1.12.** Let the position process \( x(t) \in \mathbb{R}^n \) and the inter-collision times be 2nd order Gamma distributed. Then at the collision time \( t \)

\[
\begin{align*}
E \left[ \frac{\Delta^+ x(t)}{\tau_2} | x(t) \right] &= b^+(x(t), t), \\
E \left[ \frac{\Delta^- x(t)}{\tau_1} | x(t) \right] &= b^-(x(t), t), \\
E \left[ \left( \frac{\Delta^+ x(t)}{\tau_2} \right)^2 | x(t) \right] &= b^+(x(t), t)^2 + 2\sigma^2 \frac{\tau}{\tau}, \\
E \left[ \left( \frac{\Delta^- x(t)}{\tau_1} \right)^2 | x(t) \right] &= b^-(x(t), t)^2 + 2\sigma^2 \frac{\tau}{\tau},
\end{align*}
\]

where \( \tau = 2/\beta \) is the mean inter-particle collision time and \( \epsilon = \sigma^2/M \) is the diffusion per unit mass.

**Proof.** The expectations are straightforward as the terms on the righthand side of the second and third equation in (1.22) are finite curtesy of the fact that

\[
\begin{align*}
E \left[ \frac{\Delta^+ z}{\tau_2} \right]^2 &= E \left[ \frac{1}{\tau_2} \right] = \frac{2}{\tau}, \\
E \left[ \frac{\Delta^- z}{\tau_1} \right]^2 &= E \left[ \frac{1}{\tau_1} \right] = \frac{2}{\tau},
\end{align*}
\]

The equality in the first equation in (1.21) is due to the fact that

\[
\int_{-\infty}^{\infty} (b^+(x, t) - b^-(x, t)) \rho(x, t) = \int_{-\infty}^{\infty} \left( \frac{\rho_x(x, t)}{\rho(x, t)} \right) \rho(x, t) = 0,
\]

so that the average velocity of the main particle is the same whether a forward or backward view is developed. □
Remark 1.13. As a result of (1.22) the forward and backward energy for the main particle can be defined as

\[
\mathcal{H}_M^+(x(t), t) = \frac{M}{2} E \left[ \left( \frac{\Delta^+ x(t)}{\tau_2} \right)^2 \right] = \frac{M}{2} b^+(x(t), t)^2 + \frac{\epsilon}{\tau},
\]

\[
\mathcal{H}_M^-(x(t), t) = \frac{M}{2} E \left[ \left( \frac{\Delta^- x(t)}{\tau_2} \right)^2 \right] = \frac{M}{2} b^-(x(t), t)^2 + \frac{\epsilon}{\tau},
\]

because \( \frac{M}{\tau^2} 2\sigma^2/\tau = \epsilon/\tau \).

Remark 1.14. Recall that it was assumed that \( t \gg \tau \) otherwise \( \tau_1 \) is not sufficiently close to a 2nd order Gamma distribution.

Remark 1.15. In the typical stochastic mechanics setting, \( \sigma^2 = \hbar/M \) so that the backward and forward energies have a drift component and depend on a constant equal to \( \hbar/\tau \). Typically in molecular applications at room temperatures \( M b^+(x(t), t)^2 \gg \hbar/\tau \) and only at lower temperatures \( M b^+(x(t), t)^2 \sim \hbar/\tau \). However in other applications like astrophysics or economics it remains to be seen what the drift energy is in proportion to the diffusion energy. In the molecular-kinetic theory of heat the diffusion coefficient equals \( \sigma \) so the drift energy is in proportion to the diffusion energy. In the molecular-kinetic theory of heat the diffusion energy ratio then depends on the temperature \( T \) and the viscosity \( \eta_v \).

The following example demonstrates a consequence of Theorem 1.17 and equations (1.2a) and (1.18c). Consider a Brownian particle that arrived in \( x(t) = x \) and assume that the collisions occur closely in time so \( \tau_2 \) and \( \tau_1 \) are small. From (1.18c) follows that the forward and drift for Brownian motion are determined as \( b^+(x, t) = 0 \) and \( b^-(x, t) = -x(t)/t \). The approximate energy gain or loss for the main particle can now be approximated from the outgoing and incoming energies around the collision point so in one dimension

\[
2 \left( \mathcal{H}_M^+(x(t), t) - \mathcal{H}_M^-(x(t), t) \right) = M \frac{x(t + \tau_2) - x(t)}{\tau_2} - M \frac{x(t) - x(t - \tau_1)}{\tau_1}^2,
\]

where \( \mathcal{H}_M^+(x(t), t) - \mathcal{H}_M^-(x(t), t) \) is the energy gain or loss due to the collision in \( x(t) \) at time \( t \).

Averaging over all collision points this reduces to

\[
2E \left[ \mathcal{H}_M^+(x(t), t) - \mathcal{H}_M^-(x(t), t) \right] = ME \left[ \left( \frac{\Delta^+ x(t)}{\tau_2} \right)^2 \right] - ME \left[ \left( \frac{\Delta^- x(t)}{\tau_1} \right)^2 \right]
\]

\[
= 2M \frac{\sigma^2}{\tau} - ME \left[ \frac{x(t)^2}{t^2} \right] - 2M \frac{\sigma^2}{\tau} = -\frac{M \sigma^2}{2t}.
\]

The expectation includes all paths emanating from the origin so this suggests that the main particle sheds energy continually. The expression does not depend on the mean inter-particle collision time or relates in any other way to the characteristics of the impacting particles. In fact the large contributions of the diffusion terms in the backward and forward momenta cancel exactly leaving the time dependent drift \(-M \sigma^2/(2t)\).
Equation (1.24) should have a more complicated appearance to reflect the discreteness of equation (1.2a). However, for sufficiently small \( \tau \) the conclusion must be that a particle following a Brownian motion path must be flooding its surrounding heatbath with energy thereby raising its temperature. In the continuous representation the energy transfer is infinite at the origin which is an unrealistic physical anomaly due to the discreteness of equation (1.2a). It is clear that a continual energy exchange is possible (viz. high energy protons fired into a plasma torus) but it is unexpected that a Brownian (main) particle is not in equilibrium with its surroundings.

If not Brownian Motion then the question is what stochastic process describes the equilibrium motion of the main particle in a heatbath such that there is no energy exchange between main particle and heatbath? To answer this question the next Section shows that the main particle equilibrium motion is related to the total energy conservation and investigates the constraints on the probability density function for the position of the main particle.

2. Energy Conservation

This Section combines the properties of elastic collisions to show that the main particle plus heatbath particle kinetic energy equals a quadratic expression of the backward and forward velocities. From this it is shown that if the main particle is in equilibrium with the heatbath then there is only one acceptable probability density for the position of the main particle. Another conclusion in this Section is that the forward and backward velocities of the main particle through a collision point can only be independent if the heatbath particle motion through the collision is highly correlated. Examples are presented in the form of the Gaussian Wave packet and Brownian motion.

To analyze the energy exchange associated with the collisions consider an elastic two-particle collision in \( n \) (typically 2 or 3) dimensions at time \( t \) between the main particle of mass \( M \) and the heatbath particle \( m \) where typically \( M > m \). The main particle has pre- and post-collision velocities \( v_2, v_1 \in \mathbb{R}^n \) while the heatbath particle has pre- and post-collision velocities \( w_2, w_1 \in \mathbb{R}^n \) respectively. By assumption the particles exchange energy and momentum during the collision hence \( v_2 \neq v_1 \) and \( w_2 \neq w_1 \). As there are no other interactions, the momentum and the energy during the collision must be conserved so that

\[
p_2 + q_2 = Mv_2 + mw_2 = p_1 + q_1 = Mv_1 + mw_1,
\]

\[
\frac{1}{2} (M |v_2|^2 + m |w_2|^2) = \frac{|p_2|^2}{2M} + \frac{|w_2|^2}{2m}
\]

\[
= \frac{1}{2} (M |v_1|^2 + m |w_1|^2) = \frac{|p_1|^2}{2M} + \frac{|w_1|^2}{2m}.
\]

To obtain a full solution to equation (2.1) assume a linear relationship between the main pre- and post-collision particle velocities \( v_1, v_2 \in \mathbb{R}^n \) and the incident pre- and post-collision particle velocities \( w_1, w_2 \in \mathbb{R}^n \) as follows

\[
\begin{pmatrix}
v_2 \\
w_2
\end{pmatrix} = \begin{pmatrix}
P & Q \\
V & G
\end{pmatrix} \begin{pmatrix}
v_1 \\
w_1
\end{pmatrix} = \Gamma \begin{pmatrix}
v_1 \\
w_1
\end{pmatrix},
\]

where \( P = P(x, t), Q = Q(x, t), V = V(x, t) \) and \( G = G(x, t) \) are \( \mathbb{R}^n \times \mathbb{R}^n \) matrices so that \( \Gamma = \Gamma(x, t) \) is a \( \mathbb{R}^{2n} \times \mathbb{R}^{2n} \) matrix. The following theorem determines the
form of the matrices \(P, Q, V\) and \(G\) under the conservation of energy and momentum constraints (2.1).

**Theorem 2.1.** Assume that the \(\Gamma\) matrix in (2.2) can be decomposed as 
\[
\Gamma = \begin{pmatrix} P & Q \\ V & G \end{pmatrix},
\]
then the energy and momentum conservation in (2.1) is equivalent to
\[
\begin{align*}
\Gamma^T \begin{pmatrix} M \\ m \end{pmatrix} &= \begin{pmatrix} M \\ m \end{pmatrix}, \\
\Gamma^T \begin{pmatrix} M & 0 \\ 0 & m \end{pmatrix} \Gamma &= \begin{pmatrix} M \\ 0 & m \end{pmatrix},
\end{align*}
\]
(2.3)
or equivalently
\[
\begin{align*}
P^T M + R^T m &= M, \\
Q^T M + S^T m &= m, \\
P^T M Q + V^T m G &= 0.
\end{align*}
\]
(2.4a)
(2.4b)
(2.4c)

If \(M = M I, m = m I\) (\(I\) being the unit matrix) then these equations can be solved to yield
\[
\begin{align*}
P &= \frac{\sin(\theta)}{2\gamma} \begin{pmatrix} I - \gamma^2 U \end{pmatrix}, \\
Q &= \frac{\gamma \sin(\theta)}{2} \begin{pmatrix} I + U \end{pmatrix}, \\
V &= \frac{\sin(\theta)}{2\gamma} \begin{pmatrix} I + U \end{pmatrix}, \\
G &= \frac{\gamma \sin(\theta)}{2} \begin{pmatrix} I - \frac{1}{\gamma^2 U} \end{pmatrix}, \\
U^T U &= I,
\end{align*}
\]
(2.5)
where \(U\) is an arbitrary \(n \times n\) unitary matrix \(U^T U = I\).

**Proof.** A straightforward but lengthy proof for this can be found in Appendix B. \(\square\)

**Remark 2.2.** Notice that \(Q = \gamma^2 V, P + Q = I\) and \(V + G = I\) so the collision matrix \(\Gamma(x,t)\) can be easily expressed in terms of the matrix \(Q\).

**Remark 2.3.** The matrix \(\Gamma(x,t)\) in (2.2) consists of all center of mass collision information to translate the pre-collision velocities \(v_1, w_1\) information into the post-collision \(v_2, w_2\) configuration. In one dimension this matrix is naturally absent and in higher dimensions the matrix varies randomly from collision to collision. The matrix depends on \(\Gamma = \Gamma(x,t,Z)\) where \(Z\) is an asymmetric matrix \(Z = I - 2 (I + U)^{-1}\) with \(U\) defined in (2.5). The matrix \(Z\) will be referred to as the collision scattering matrix. With elastic collisions this matrix is independent of the energy pre-collision energy \(v_1\) and \(w_1\) and typically reflects the physical circumstances of the collision event.

For \(U = I, Z \equiv 0\), equation (2.5) reduces to a simpler set of linear equations which shall be referred to as the "simple" elastic collision
\[
\begin{pmatrix} v_2 \\ w_2 \end{pmatrix} = \begin{pmatrix} \cos(\theta) I & \gamma \sin(\theta) I \\ \sin(\theta) I & -\cos(\theta) I \end{pmatrix} \begin{pmatrix} v_1 \\ w_1 \end{pmatrix} = \Omega \begin{pmatrix} v_1 \\ w_1 \end{pmatrix},
\]
(2.6)
with obvious definition of the matrix \(\Omega\) and \(I\) being the unit matrix in \(n\) dimensions. Here \(\gamma = \frac{m}{M}, \cos(\theta) = \frac{1 - \gamma^2}{1 + \gamma^2}, \sin(\theta) = \frac{2v_1}{1 + \gamma^2}.\) In one dimension this solution is unique as in that case \(Z \equiv 0\). This expression also applies if \(\gamma = 1 (m = M)\) in which case the particles simply exchange velocities \(v_2 = w_1, w_2 = v_1\). The matrix \(\Omega\) is
a reflection transformation with $\det(\Omega) = -1$, $\Omega^T \Omega = I$, Trace$(\Omega) = 0$ and has eigenvectors

$$
\begin{pmatrix}
\cos(\frac{\theta}{2}) \\
\sin(\frac{\theta}{2})
\end{pmatrix}, \begin{pmatrix}
sin(\frac{\theta}{2}) \\
-\cos(\frac{\theta}{2})
\end{pmatrix},
$$

with eigenvalues 1, -1. Notice also that $\cos(\theta/2) = \frac{1}{1+\gamma^2}$ and $\sin(\theta/2) = \frac{\gamma}{1+\gamma^2}$.

**Remark 2.4.** Equation (2.6) has a unique solution in the sense that the main and heatbath particle exchange momentum and energy along the center of mass line at the moment of collision while other components of the motion remain invariant. This means that in higher dimensions equation (2.6) applies to the pre- and post-collision velocity components of $v_2, w_2, v_1, w_1$ along the center of mass line. The components of $v_1$ and $w_1$ orthogonal to the collision center of mass line remain invariant under an elastic collision. In this Section no real distinction is made between the properties of the heatbath particle and the properties of its center of mass line components.

A simple theorem now describes how the energy conservation for the motion for the heatbath particle $m, w_1$ (post-collision $m, w_2$) and the main particle $M, v_1$ (post-collision $M, v_2$) can be expressed exclusively in terms of $v_2$ and $v_1$ if (2.6) holds.

**Theorem 2.5.** Let the momentum of the main particle and interacting particle be presented as $p_1 = Mv_1$ (post-collision $p_2 = Mv_2$) and $q_1 = Mw_1$ (post-collision $q_2 = Mw_2$) with $v_1, v_2, w_1, w_2 \in \mathbb{R}^n$. Then the total energy $\mathcal{H}_T = \frac{1}{2}(Mv_2^2 + mw_2^2) = \frac{1}{2}(Mv_1^2 + mw_1^2)$ is related to the pre- and post collision of momenta of the main particle as follows:

$$
\frac{M\gamma^4}{1+\gamma^2} \mathcal{H}_k = \frac{1}{2} \left| \frac{q_2 + q_1}{2} \right|^2 + \frac{\gamma^2}{2} \left| \frac{q_2 - q_1}{2} \right|^2,
$$

for the heatbath particle, while for the main particle

$$
\frac{M}{1+\gamma^2} \mathcal{H}_k = \frac{1}{2} \left| \frac{p_2 + p_1}{2} \right|^2 + \frac{1}{2\gamma^2} \left| \frac{p_2 - p_1}{2} \right|^2.
$$

In terms of the velocities these equations become

$$
\mathcal{H}_k = \frac{1}{2} \left| \frac{w_2 + w_1}{2} \right|^2 + \frac{\gamma^2}{2} \left| \frac{w_2 - w_1}{2} \right|^2, \quad (2.7a)
$$

$$
\mathcal{H}_k = \frac{1}{M_T^2} \left| \frac{v_2 + v_1}{2} \right|^2 + \frac{1}{2\gamma^2} \left| \frac{v_2 - v_1}{2} \right|^2, \quad (2.7b)
$$

with $M_T = M + m = M(1 + \gamma^2)$. Also a more direct relationship between the momenta can be derived as follows

$$
\left| \frac{v_2 + v_1}{2} \right|^2 + \frac{1}{\gamma^4} \left| \frac{v_2 - v_1}{2} \right|^2 = \frac{1}{2} |w_1|^2 + |w_2|^2. \quad (2.7b)
$$

Proof. See Appendix A. □

**Remark 2.6.** The previous remark (2.4) implies that in higher dimensions equations (2.7a) and (2.7b) apply to the center of mass line components of the main and heatbath particles. In other words if $n > 1$ the kinetic energy $\mathcal{H}_k$ incorporates only the parts of the motion of the heatbath particle that are altered due to the collision.
The motion perpendicular to the center of mass line remains invariant hence this energy component remains the same and must be added to $\mathcal{H}_k$ in order to derive the full energy of the heatbath and main particle combined. In Section 4 equations (2.7a) and (2.7b) will be investigated for the case where $Z \neq 0$ so there $\mathcal{H}_k$ will represent the combined kinetic energy.

Remark 2.7. It deserves mentioning that equations (2.7a) and (2.7b) only hold for a collision point and are in fact incorrect for any intermediate points.

Conceptually equation (2.7a) suggests that the fracturing of the path of the main particle provides a direct indication of the amount of energy that is involved in the main and heatbath particle system combined. Moreover, condition (2.7b) is independent of the energy constraint (2.7a) and tends to constrain the momentum exchange between the particles involved. For this reason (2.7a) is referred to as the "energy" balance/constraint and (2.7b) as the "momentum" constraint.

The agenda for further developments is now to employ the collision representation of the Markovian process describing the path of the main particle in equation (1.2a) and substitute the respective forward and backward velocities (1.3) into (2.7a). Due to the distribution of the inter-collision stopping times the expectation of the total energy components in the collision process will be well defined. The mean inter-particle collision is small so the use of equation (1.2b) is well justified. The total energy as a function of time and position can then be investigated.

First an important consequence of equation (2.2) must be noted. Rewrite equation (2.6) so as to represent the pre- and post-collision velocities of the main particle as a function of the velocities of the colliding heatbath particle. This shows that

$$
\begin{pmatrix} v_2 \\
v_1 \end{pmatrix} = \frac{\gamma}{\sin(\theta)} \begin{pmatrix} 
\cos(\theta) & I \\
I & \cos(\theta) I \end{pmatrix} \begin{pmatrix} w_2 \\
w_1 \end{pmatrix},
$$

hence the statistical properties of $v_2, v_1$ are generated by the behavior of $w_2, w_1$ and vice versa.

Specifically equations (1.2a) and (1.2b) demand that the motion of the heatbath particle must be of the following form

$$
w_2 = g^+(x(t), t) + \omega \frac{\Delta^+}{\tau_2},$$

$$w_1 = g^+(x(t), t) + \omega \frac{\Delta^+}{\tau_1},$$

which substituted into equation (2.8) yields

$$
\begin{pmatrix} b^+(x(t), t) + \sigma \frac{\Delta^+ z}{\tau_2} \\
b^+(x(t), t) + \sigma \frac{\Delta^+ z}{\tau_1} \end{pmatrix} = \cos(\theta) \begin{pmatrix} b^-(x(t), t) + \sigma \frac{\Delta^- z}{\tau_1} \\
b^-(x(t), t) + \sigma \frac{\Delta^- z}{\tau_1} \end{pmatrix} \\
+ \gamma \sin(\theta) \begin{pmatrix} g^-(x(t), t) + \omega \frac{\Delta^+}{\tau_1} \\
g^-(x(t), t) + \omega \frac{\Delta^+}{\tau_1} \end{pmatrix},
$$

$$
\begin{pmatrix} g^+(x(t), t) + \sigma \frac{\Delta^+ w}{\tau_2} \\
g^+(x(t), t) + \sigma \frac{\Delta^+ w}{\tau_1} \end{pmatrix} = \frac{\sin(\theta)}{\gamma} \begin{pmatrix} b^-(x(t), t) + \sigma \frac{\Delta^- z}{\tau_1} \\
b^-(x(t), t) + \sigma \frac{\Delta^- z}{\tau_1} \end{pmatrix} \\
- \cos(\theta) \begin{pmatrix} g^-(x(t), t) + \omega \frac{\Delta^- w}{\tau_1} \\
g^-(x(t), t) + \omega \frac{\Delta^- w}{\tau_1} \end{pmatrix},
$$
or equivalently

\[
\begin{pmatrix}
    b^+(x(t), t) \\
    b^-(x(t), t)
\end{pmatrix} = \frac{\gamma}{\sin(\theta)} \begin{pmatrix}
    \cos(\theta) & 1 \\
    1 & \cos(\theta)
\end{pmatrix} \begin{pmatrix}
    g^+(x(t), t) \\
    g^-(x(t), t)
\end{pmatrix},
\]

(2.9a)

\[
\begin{pmatrix}
    \sigma \Delta^+_{\tau_2} \\
    \sigma \Delta^-_{\tau_1}
\end{pmatrix} = \frac{\gamma}{\sin(\theta)} \begin{pmatrix}
    \cos(\theta) & 1 \\
    1 & \cos(\theta)
\end{pmatrix} \begin{pmatrix}
    \omega \Delta^+_{\tau_2} \\
    \omega \Delta^-_{\tau_1}
\end{pmatrix}.
\]

(2.9b)

Hence the motion of the heatbath particle must be driven by backward and forward drifts \( g^\pm(x, t) \) and corresponding random impulses \( \omega \Delta^\pm_{\tau_2}, \omega \Delta^\pm_{\tau_1} \). As subsequent collisions involve different heatbath particles the realizations from the heatbath particles \( w_1, w_2 \) should be the result of a time dependent random field. Specifically the post-collision heatbath velocity \( w_2(x(t), t) \) for the collision at \( x(t), t \) is not equal to the pre-collision velocity \( w_1(x(t + \tau_2), t + \tau_2) \) as they involve different particles. No continuity equation therefore applies to \( g^\pm(x, t) \). However equations (2.9a) and (2.9b) show that the heatbath realizations are constrained by the motion of the main particle.

The other important consequence of (2.9b) is that the main particle forward and backward velocities \( \Delta^+z, \Delta^-z \) can only be independent if the heatbath particle forward and backward velocities \( \Delta^+_w, \Delta^-_w \) are appropriately correlated. The following Theorem details the autocorrelation in the heatbath particle motion and also shows that the random terms \( \Delta^+_w, \Delta^-_w \) must be cross correlated with \( \Delta^+_z, \Delta^-_z \).

**Theorem 2.8.** If the main particle follows a Markovian path i.e if \( \Delta^+z, \Delta^-z \) in equation (2.9b) are uncorrelated, then \( \omega^2 = \frac{\sigma^2}{2\alpha^2} \), where \( \alpha^2 = \frac{\gamma^4}{1 + \gamma^4} \). Also the \( \Delta^+_w, \Delta^-_w \) must be correlated as

\[
\text{corr} \left( \frac{\Delta^+_{\tau_2}}{\tau_2}, \frac{\Delta^-_{\tau_1}}{\tau_1} \right) = - \left( 1 - 2\alpha^2 \right).
\]

If \( m << M \) then \( \alpha \) is very small hence the variance term \( \omega \) must be large and the correlation between the pre-collision and post-collision velocities of the heatbath particle must be very high.

In addition the forward and backward velocities of the main and incident particle have covariances

\[
\begin{align*}
E \left[ \frac{\Delta^+_w \Delta^+_z}{\tau_2^2} \right] &= E \left[ \frac{\Delta^-_w \Delta^-_z}{\tau_1^2} \right] = - \frac{\sqrt{2} \alpha}{\gamma \sin(\theta)} \cos(\theta), \\
E \left[ \frac{\Delta^+_w \Delta^-_z}{\tau_2 \tau_1} \right] &= E \left[ \frac{\Delta^-_w \Delta^+_z}{\tau_2 \tau_1} \right] = \frac{\sqrt{2} \alpha}{\gamma \sin(\theta)}.
\end{align*}
\]

**Proof.** Inverting equation (2.9b) yields

\[
\begin{pmatrix}
    \omega \Delta^+_{\tau_2} \\
    \omega \Delta^-_{\tau_1}
\end{pmatrix} = \frac{1}{\gamma \sin(\theta)} \begin{pmatrix}
    -\cos(\theta) & 1 \\
    1 & -\cos(\theta)
\end{pmatrix} \begin{pmatrix}
    \sigma \Delta^+_{\tau_2} \\
    \sigma \Delta^-_{\tau_1}
\end{pmatrix},
\]

(2.10)
and if the increments $\sigma \frac{\Delta^+}{t_2}$ and $\sigma \frac{\Delta^-}{t_1}$ are independent then

$$\omega^2 E \left[ \left( \frac{\Delta^+}{t_2} \right) \left( \frac{\Delta^-}{t_1} \right) \right]$$

$$= \frac{2\sigma^2}{\tau_2 \gamma^2 \sin^2(\theta)} \left( \begin{array}{cc} -\cos(\theta) & 1 \\ 1 & -\cos(\theta) \end{array} \right)^2$$

$$= \frac{\sigma^2}{\tau \alpha^2} \left( \begin{array}{cc} 1 & - (1 - 2\alpha^2) \\ - (1 - 2\alpha^2) & 1 \end{array} \right),$$

where $\alpha^2 = \gamma^4 / (1 + \gamma^4)$. If it is assumed that

$$E \left[ \left( \frac{\Delta^+}{t_2} \right)^2 \right] = E \left[ \left( \frac{\Delta^-}{t_1} \right)^2 \right] = \frac{2}{\tau},$$

then $\omega = \sigma / (\alpha \sqrt{2})$ and the correlation follows directly.

Using (2.10) again it is also clear that

$$\omega \sigma E \left[ \left( \frac{\Delta^+}{t_2} \right) \left( \frac{\Delta^-}{t_1} \right) \right]$$

$$= \frac{2\sigma^2}{\tau_2 \gamma \sin(\theta)} \left( -\cos(\theta) \\ 1 \right) \left( 1 - \cos(\theta) \right),$$

so that

$$E \left[ \left( \frac{\Delta^+ \Delta^z}{t_2} \right) \left( \frac{\Delta^- \Delta^-}{t_1} \right) \right]$$

$$= \frac{\sqrt{2}\alpha}{\gamma \sin(\theta)} \left( -\cos(\theta) \\ 1 \right) \left( 1 - \cos(\theta) \right),$$

which concludes the proof. \qed

**Remark 2.9.** If $\gamma << 1$ then the $\omega^2$ variance term becomes very large and the correlation between $\sigma \frac{\Delta^+}{t_2}$ and $\sigma \frac{\Delta^-}{t_1}$ becomes tighter. In the limit where $\gamma \approx 0$, e.g. a football interacting with molecules or a planet interacting with cosmic particles (or photons) a small diffusion constant $\sigma$ for the main object is associated with an enormous heatbath particle momentum proportional to $\sigma / (\alpha \sqrt{2})$. In this case the post-collision heatbath particle velocity size is identical to the pre-collision heatbath velocity but moving in the opposite direction.

The next issue to investigate is the total kinetic energy $\mathcal{H}_k$ in (2.11) as a function of time while the main particle travels from collision to collision. By assumption the collision is elastic and conserves the total energy so if $w_1$ and $w_2$ refer to the same particle (the first one before the collision and the second one after the collision with the main particle) then by definition

$$\mathcal{H}_k = \mathcal{H}_k(x(t), t) = \frac{1}{2} M |v_1|^2 + \frac{1}{2} m |w_2|^2$$

$$= \frac{1}{2} M |v_1|^2 + \frac{1}{2} m |w_2|^2.$$




However, for the subsequent collision the main particle moving with momentum $Mv_2$ will meet a different heat bath particle at time $t + \tau_2$ in a new position $x(t + \tau_2) = x(t) + b^\dagger(x, t)\tau_2 + \sigma^\dagger z(t)/\tau_2$. This new heat bath particle will have a new momentum $mv'$ which is chosen randomly from the ensemble. Obviously the exiting total kinetic energy at $x(t)$ and the combined ”new” total kinetic energy at $x(t + \tau_2)$ will not be equal since

$$H_k'(x(t + \tau_2), t + \tau_2) = \frac{1}{2}M|v_2|^2 + \frac{1}{2}m|q'|^2 
\neq \frac{1}{2}M|v_2|^2 + \frac{1}{2}M|w_2|^2.$$

Hence that the combined system (main + heat bath particle) gains or loses energy $\Delta H_k(x(t), t)$ equal to

$$\Delta H_k(x(t), t) = H_k(x(t + \tau_2), t + \tau_2) - H_k(x(t), t) = \frac{m}{2}(|q|^2 - |w_2|^2).$$

On average the amount of energy exchanged equals

$$E[\Delta H_k(x(t), t)] = \frac{m}{2}E[|q|^2] - \frac{m}{2}E[|w_2|^2] \quad (2.11)$$

where the expectation $\bar{q}E[|q|^2]$ is the average energy of the new incoming heat bath particle at collision time $t + \tau_2$ and $\frac{m}{2}E[|w_2|^2]$ is the post collision energy of the previous heat bath particle at the previous collision time $t$. The expectation here is over all paths, heat bath interactions and all positions $x(t)$.

If $(2.11)$ is positive the original post collision energy of the heat bath particle at $t$ has a lower energy than the new heat bath particle colliding at $t + \tau_2$ and if this quantity is negative the collision accelerated the heat bath particle coming out of $x(t)$ in comparison to the typical heat bath particle. In the first case the colliding heat bath particle returned to the heat bath with less energy than the average heat bath particle and in the second case the collision accelerated the colliding heat bath particle beyond the heat bath average. If $(2.11)$ is positive the heat bath puts energy into the main particle lowering its temperature and if $(2.11)$ is negative the main particle radiates energy into the heat bath thereby heating it up. Changes in the expected total energy along the path of the main particle therefore show the amount of energy that is being exchanged between main particle and heat bath.

The important result is that if the main particle resides in heat bath equilibrium the expectation $(2.11)$ should be zero. In other words if the main particle does not radiate energy into the heat bath, if the main particle movement has adopted the heat bath temperature then the total kinetic energy $H_k$ must be a conserved quantity. If radiation occurs in the form of an energy exchange between main particle and heat bath then there must a potential or explanatory term describing the additional physical process. In this case it must be assumed that the total kinetic energy and the potential term together are conserved.

Assume therefore a static potential $\Phi_p \in \mathbb{R}, \Phi : \mathbb{R} \times [0, \infty] \rightarrow \mathbb{R}$ such that the (average) energy exchange can be related to $(2.11)$ as

$$E[\Phi_p(x(t + \tau_2), t + \tau_2)] - E[\Phi_p(x(t), t)] = -\frac{m}{2}E[|q|^2] + \frac{m}{2}E[|w_2|^2], \quad (2.12)$$
then
\[ E[\mathcal{H}_k(x(t + \tau_2), t + \tau_2) - \mathcal{H}_k(x(t), t)] = -(E[\Phi_p(x(t + \tau_2), t + \tau_2)] - E[\Phi_p(x(t), t)]). \]

Defining the total energy of main and heatbath particle as \( \mathcal{H}_T(x(t), t) = \mathcal{H}_k(x(t), t) + \Phi_p(x(t), t) \) then (2.13) implies that \( E[\mathcal{H}_T(x(t + \tau_2), t + \tau_2)] = E[\mathcal{H}_T(x(t), t)] \). In other words the Hamiltonian \( E[\mathcal{H}_T(x(t), t)] \) must be time invariant. The expectation \( E[\mathcal{H}_k(x(t), t)] \) is the kinetic energy term associated with the motion (of both the main and incident particle) and \( \Phi_p \) is the static potential energy term that regulates the energy exchange between heatbath and main particle.

Using Theorem (2.2), definition (1.2) and approximation (1.2b) it is possible to provide more detail on the precise form of the total energy total energy \( \mathcal{H}_T \).

**Proposition 2.10.** Let the average velocity of the main particle be defined as
\[ \overline{v} = \overline{v}(x,t) = \frac{b^+(x(t), t) + b^-(x(t), t)}{2}, \]
then in \( n \) dimensions the expectation of the total energy \( E[\mathcal{H}_T] \) can be written as
\[ E[\mathcal{H}_T] = E[\mathcal{H}_k + \Phi_p] = \frac{M_T}{2} E[\overline{v}(x(t), t)]^2 + \frac{M_T \sigma^2}{8 \gamma^2} E\left[ \frac{1}{\rho} |\nabla \rho|^2 \right] \]
\[ + E[\Phi_p(x(t), t)] + \frac{2n \epsilon}{\sin^2(\theta) \gamma}, \]
with \( M_T = M + m, \sigma^2 = \frac{1}{\gamma} \). Here \( \rho(x,t) \) is the probability density function for \( x(t) \) and the potential \( \Phi_p \) is defined in (2.14).

**Proof.** The terms that requires an explanation are the expectation of the kinetic energy term \( \mathcal{H}_k \) and the resident constant. Using (2.1a) this expectation reduces to
\[ E\left[ \frac{\mathcal{H}_k}{M_T} \right] = \frac{1}{2} E \left[ \frac{v_x^2 + v_y^2}{2} + \frac{1}{\gamma^2} \left| \frac{v_x - v_y}{2} \right|^2 \right] \]
\[ = \frac{1}{2} E \left[ \overline{v}(x(t), t) + \frac{1}{\gamma^2} \left| \frac{\Delta^z - \Delta^- z}{\tau_2} \right|^2 \right] \]
\[ + \frac{1}{2 \gamma^2} E \left[ \frac{b^+(x(t), t) - b^-(x(t), t)}{2} + \frac{1}{\gamma^2} \left| \frac{\Delta^z - \Delta^- z}{\tau_1} \right|^2 \right], \]
which can be simplified to
\[ E\left[ \frac{\mathcal{H}_k}{M_T} \right] = \frac{1}{2} E \left[ \overline{v}(x(t), t) \right]^2 \]
\[ + \frac{1}{2 \gamma^2} E \left[ \frac{b^+(x(t), t) - b^-(x(t), t)}{2} \right]^2 + \frac{n}{2} \left( 1 + \frac{1}{\gamma^2} \right) \frac{\sigma^2}{\gamma} \]
\[ = \frac{1}{2} E \left[ \overline{v}(x(t), t) \right]^2 + \frac{\sigma^4}{8 \gamma^2} E \left[ \frac{1}{\rho} |\nabla \rho|^2 \right] \]
\[ + \frac{n \left( 1 + \gamma^2 \right) \epsilon}{2m \gamma}, \]
if \( \sigma^2 = \frac{\epsilon}{\gamma} \). Again here \( \rho(x, t) \) is the probability density for \( x(t) \) used in equation (1.24) to find an expression for the \( b^+ (x(t), t) - b^- (x(t), t) \) term.

The constant in \( E[\mathcal{H}_b] / M_T \) is the result of the fact that

\[
\frac{1}{2} \left( 1 + \frac{1}{\gamma^2} \right) \sigma^2 = \frac{1}{2} \left( 1 + \frac{1}{\gamma^2} \right) \frac{\epsilon}{M_T} = \frac{(1 + \gamma^2) \epsilon}{2\gamma^2 M_T} = \frac{(1 + \gamma^2) \epsilon}{2m\gamma},
\]
a constant depending only on the properties of the incident particles. This means that

\[
E[\mathcal{H}_b] \sim nM_T \left( 1 + \gamma^2 \right) \epsilon = \frac{n(1 + \gamma^2)^2 \epsilon}{2\gamma^2} = \frac{2n\epsilon}{\sin(\theta)^2\gamma},
\]

which explains the constant in (2.14). This reconciles all the terms and the Theorem is proved.

**Remark 2.11.** Comparing the diffusion energy term \( \epsilon/\gamma \) in (1.23) it is clear that the diffusion energy for the total kinetic energy \( \frac{2n\epsilon}{\sin(\theta)^2\gamma} \) in Proposition 2.10 above is much larger if \( \gamma << 1 \). This is due to the presence of the heatbath particle diffusion energy.

The radiation requirement introduced above imposes a restriction on the distribution density for the position of the main particle. This result is summarized in the following Theorem.

**Theorem 2.12.** Let the potential \( \Phi_p : \mathbb{R} \times [0, \infty] \rightarrow \mathbb{R} \) defined in equation (2.10) be such that

\[
\frac{d}{dt} E[\Phi_p (x(t), t)] = E \left[ \frac{b^+ + b^-}{2} \right] \nabla \phi,
\]

for a suitable potential \( \phi : \mathbb{R} \times [0, \infty) \rightarrow \mathbb{R} \) which is at least once differentiable. Then the only probability density distribution \( \rho(x, t) \) for the main particle position process \( x(t) \) that allows the total energy \( E[\mathcal{H}_b] = E[\mathcal{H}_b + \Phi_p] \) defined in Proposition 2.10 to be time invariant is derived from the wave function \( \psi(x, t), x \in \mathbb{R}, t \in [0, \infty), \psi : \mathbb{R} \times [0, \infty) \rightarrow \mathbb{C} \) such that \( \rho(x, t) = |\psi(x, t)|^2 \), where the wave function satisfies Schrödinger’s equation

\[
i\chi \psi(x, t)_t = -\frac{\chi^2}{2M_T} \Delta_x \psi(x, t) + \phi(x, t) \psi(x, t),
\]

with \( \chi = M_T \eta = M_T \sigma^2 = \left( \gamma + \frac{1}{\gamma} \right) \epsilon / \sin(\theta) \) and \( \Delta_x = \left( \frac{\partial^2}{\partial x_1^2}, \ldots, \frac{\partial^2}{\partial x_n^2} \right) \). If the wave function is written as \( \psi = \psi(x, t) = e^{iR(x, t) + S(x, t)} \) then the forward and backward drift can be written as

\[
b^+ (x, t) = \frac{1}{M_T} (\nabla S + \gamma \nabla R) = \frac{\chi}{M_T} (\text{Im} \pm \text{Re}) \frac{\nabla \psi(x, t)}{\psi(x, t)}.
\]

The constant total energy now equals

\[
E[\mathcal{H}_b] = \frac{\chi^2}{2M_T} E[|\nabla \psi|^2] + E[\Phi_p] + \frac{2n\epsilon}{\sin^2(\theta)\gamma}.
\]
Proof. The proof here is part of a more general result presented in Appendix C. Nelson [8] showed the relationship between the wave function and an energy functional similar to (2.14). In Nelson [7] this result was extended to incorporate a potential term as introduced in (2.12) though condition (2.16) is different. The proof in Appendix C is for a more general energy expression incorporating the presence of the collision scattering matrix $Z$ but runs similar to the presentation in Nelson [7]. Carlen [12] demonstrated that the stochastic differential equation (1.8) admits a weak solution if the potential $\phi(x, t)$ belongs to a class Kato-Rellich potential. □

Remark 2.13. Equation (2.19) above incorporates the total energy of the system, i.e. the energy of the main particle as well as the energy of the incident particle. The mass in the equation refers to the combined mass of the system $M_T = M + m$ rather than the main particle and it is not specified how this energy is distributed between the two particles.

Remark 2.14. Under conditions (1.5), (1.6) and sufficiently small $\tau$ the discrete collision process (1.2a) can be approximated by the continuous stochastic differential equation (1.8). Hence both the momenta and (forward and backward) energies (1.3) can be approximated using (2.18) see Carlen [13]. As a result $H_T$ in (2.14) is now a well defined estimate of the combined energy.

There is no reference in this approach to quantum mechanics or a stochastic interpretation of quantum mechanics. Though the proof in Appendix B is quite similar to the stochastic mechanics approach presented in Nelson [7], Theorem (2.12) above does not reproduce an interpretation of quantum mechanics at least not perfectly as the scaling here is different. Obviously, if Planck’s constant were chosen as $\hbar = \chi$ then (2.17) reduces to the wave-function for a particle, however, the forward and backward drifts in (2.18) explode if the mass ratio $\gamma$ were allowed to approach zero. In addition the mass term $M_T$ incorporates information on both the main and heatbath particle and the energy (2.19) refers to the combined kinetic and potential energy.

2.1. The Brownian Motion. This continued example demonstrates what happens to the total kinetic energy for a particle following a Brownian motion if no conservation law applies. The Gaussian distribution is the result of the diffusion equation with a zero forward drift $b^+(x, t)$ so that the probability density and backward drift equal

$$
\rho(x, t) = \frac{1}{\sigma \sqrt{2\pi t}} e^{-\frac{(x-\mu)^2}{2\sigma^2 t}},
$$

$$
b^-(x, t) = \frac{(x - \mu)}{t},
$$

then equation (2.15) reduces to

$$
E[H_k] = M_T E \left[ |x - \mu|^2 \right] \left( 1 + \gamma^2 \frac{t}{2\sigma^2} \right) + M_T \epsilon \frac{t}{2\sigma m} \equiv M_T \sigma^2 \left( 1 + \gamma^2 \right) + M_T \epsilon \frac{t}{2\sigma m} = \frac{\epsilon}{4 \gamma \sin(\theta) \tau} \left( 1 + 4 \frac{\tau}{nt} \right),
$$
so the total energy in classical diffusion decreases continuously though there is no evidence of a potential. Applying (2.11) shows that

\[
E \left[ \Delta H_k(x(t), t) \right] = E \left[ H_k(x(t + \tau_2), t + \tau_2) - H_k(x(t), t) \right] = \frac{\epsilon}{\gamma \sin(\theta) n} E \left[ \frac{1}{(t + \tau)} - \frac{1}{t} \right] = -\frac{\epsilon \gamma}{\gamma \sin(\theta) m T^2},
\]

which implies that a particle following a Brownian path always radiates energy into the heatbath. Brownian motion seems a non-equilibrium solution and a main particle can only perform a Brownian path due to a hidden potential that forces the motion (a dampened time-dependent oscillator would suffice). The effect mitigates quickly with time \( t \) increasing as a multiple of the collision time. In a very dense heatbath the inter-collision time shortens so for macroscopic objects the moment to equilibrium must be almost instantaneous. Notice that the effect depends on the mass ratio and is not just a function of the main particle mass \( M \).

To understand why for a Brownian Motion the average total energy changes consider that classical diffusion is a limiting case (limit in time and space dimension) of a particle stepping forward over a lattice grid with equal probability. If the process has moved a large distance to position \( x \) in a short amount of time the stochastic path of the particle has a strong backward drift in the direction of the origin. However, the forward drift is zero so for these paths the contribution to the total energy is large and ultimately too large to limit the average total energy. A path produced by a time invariant average total energy realizes that the backward drift is large and adapts the forward drift to point in a similar direction as the backward drift. Changing the drift will then reduce energy in the regions where \( x \) becomes large by reducing the acceleration.

For the next example the following Corollary will be useful.

**Corollary 2.15.** The drift for the heatbath motion is given by

\[
g^\pm(x, t) = \frac{1}{M_T} \left( \nabla S \mp \frac{1}{\gamma} \nabla R \right)
\]

so clearly

\[
g^+ (x, t) = \frac{1}{\gamma M_T \sin(\theta)} \left( \frac{1 - \cos(\theta)}{-\gamma(1 + \cos(\theta))} \nabla S \right)
\]

\[
= \frac{1}{M_T} \left( \nabla S - \frac{1}{\gamma} \nabla R \right),
\]
\[ g^-(x, t) = \frac{1}{M_T} \left( \nabla S + \frac{1}{\gamma} \nabla R \right), \]

and the Corollary is proved. \qed

**Remark 2.16.** Analogous to Lemma (1.12) and equation (1.23) the average momentum and energy for the heatbath particle can be determined as

\[
E \left[ \frac{\Delta^+ w(t)}{\tau_2} \right] x(t) = g^+(x(t), t), \quad E \left[ \frac{\Delta^- w(t)}{\tau_1} \right] x(t) = g^-(x(t), t),
\]

\[
\mathcal{H}_m^+ (x(t), t) = \frac{m}{2} E \left[ \left( \frac{\Delta^+ w(t)}{\tau_2} \right)^2 \right] x(t) = \frac{m}{2} g^+(x(t), t)^2 + \frac{\gamma^2 \epsilon}{\alpha^2 \tau}, \quad (2.20)
\]

\[
\mathcal{H}_m^- (x(t), t) = \frac{m}{2} E \left[ \left( \frac{\Delta^- w(t)}{\tau_1} \right)^2 \right] x(t) = \frac{m}{2} g^-(x(t), t)^2 + \frac{\gamma^2 \epsilon}{\alpha^2 \tau},
\]

since \( m \sigma^2 / (2 \alpha^2 \tau) = \gamma^2 \epsilon / (\alpha^2 \tau) \).

This Corollary together with (2.8) completes a description of the behavior of the main and heatbath particles. If the main particle motion behaves like a martingale where its energy exchange with the heatbath is derived from a potential \( \Phi_p \) then its probability density and (forward and backward) drifts are derived from Schrödinger’s equation (2.17) and equations (2.18). The colliding heatbath particle has a drift as specified in Corollary (2.15) and exhibits a high degree of correlation between its backward and forward momentum as shown in Theorem (2.8). The heatbath particle motion is also highly correlated with the motion of the main particle and can not be a martingale process itself.

The following example shows a solution to equations (2.17) and (2.18) for the case where the path of the main particle can be represented by a generic Gaussian process.

**2.2. The QM Wave Packet.** Applying Theorem (2.12) and Corollary (2.15) to the Gaussian function wave packet in one dimension shows that the wave function can be represented as a Gaussian superposition of single momentum solutions to the wave equation (2.17). Hence

\[
\psi(x, t) = C \int_{-\infty}^{\infty} e^{-\frac{(p-p_0)^2}{2\sigma^2}} e^{i\chi \left( px - \frac{p^2 t}{2MT} \right)} dp
\]

\[
= C \int_{-\infty}^{\infty} e^{-\frac{z^2}{2\sigma^2}} e^{i \chi \left( (z+p_0) \frac{1}{M_T} - \frac{(z+p_0)^2 t}{2MT} \right)} dz
\]

\[
= C e^{i\chi p_0 - \frac{\sigma^2}{2MT}} \int_{-\infty}^{\infty} e^{i z \mu(x, t) - \frac{z^2}{2\Gamma(t)}} dz,
\]

where

\[
\mu(x, t) = \frac{1}{\chi} \left( x - \frac{p_0 t}{M_T} \right),
\]

\[
\Gamma(t) = \frac{1}{\sigma^2} + i \frac{t}{\chi MT}.
\]
Hence
\[
\psi(x, t) = C'(t) e^{i p_0 \mu(x, t)} e^{-\frac{\mu(x, t)^2}{2 \sigma_e^2(t)}},
\]
where
\[
Z_f(t) = \Gamma(t) \Gamma(t) = \left( \frac{1}{\sigma_e^2} + \alpha^2 t^2 \right), \quad \alpha = \frac{1}{\chi M_T},
\] (2.21)
and where \( C' = \left( \sqrt{\Gamma(t)} \chi \sigma_e \sqrt{\pi} \right)^{-1} e^{\frac{x^2}{2 \sigma_e^2(t)}}. \) This constant is chosen to insure that \( \rho(x, t) = |\psi(x, t)|^2 \) is a probability density.

Rewriting \( \Gamma(t) = \sqrt{Z_f(t)}e^{i \arccos \left( \frac{\chi M}{\sqrt{Z_f(t)}} \right)} \) the wave function \( \psi(x, t) \) can be represented as
\[
\psi = \psi(x, t) = e^{i \frac{p_0 \mu(x, t)}{\chi M_T} + \chi \sigma_e^2(t)}
\]
where
\[
R(x, t) = -\left( \frac{x - \frac{p_0 t}{M_T}}{2 \chi^2 \sigma_e^2 Z_f(t)} \right)^2 - \frac{1}{2} \log \left( \chi \sigma_e \sqrt{Z_f(t)} \pi \right),
\]
\[
S(x, t) = \frac{\alpha t}{2 \chi^2 Z_f(t)} \left( x - \frac{p_0 t}{M_T} \right)^2 + \left( \frac{x_0}{\chi} - \frac{p_0^2}{2 \chi M_T} \right) - \frac{1}{2} \arccos \left( \frac{1}{\sigma_e^2 \sqrt{Z_f(t)}} \right),
\]
with \( \alpha \) and \( Z_f(t) \) as defined in (2.21). Finally, then
\[
\frac{\partial}{\partial x} R(x, t) = -\frac{\left( x - \frac{p_0 t}{M_T} \right)}{\chi^2 \sigma_e^2 Z_f(t)},
\]
\[
\frac{\partial}{\partial x} S(x, t) = \frac{\alpha t}{\chi^2 Z_f(t)} \left( x - \frac{p_0 t}{M_T} \right) + p_0.
\]
Hence \( x(t) \) is a (Gaussian) random variable such that \( E[x(t)] = \frac{p_0 t}{M_T}, \text{var}(x(t)) = Z_f(t) \chi^2 \sigma_e^2. \)

Using (2.13) the drift functions become
\[
b^\pm(x, t) = \frac{1}{\chi M_T Z_f(t)} \left( x - \frac{p_0 t}{M_T} \right) \left( \alpha t \mp \frac{\gamma}{\sigma_e^2} \right) + \frac{p_0}{M_T},
\] (2.22)
and the total energy becomes
\[
E[\mathcal{H}_k] = \frac{1}{2M_T} E \left[ R^2 + S^2 \right] + \frac{(1 + \gamma^2)^2}{2 \gamma^2 \pi} + \frac{p_0^2}{2 M_T} + \frac{2 \epsilon}{\sin(\theta) \sqrt{\pi}},
\] (2.23)
Hence the energy consists of a contribution due to the energy dispersion controlled by \( \sigma_e \), the mean kinetic energy term with \( p_0 \) and the diffusion term proportional to the variance \( \sigma^2 \).

Now the forward and backward energy (1.22) equal
\[
E \left[ \mathcal{H}_M^\pm (x(t), t) \right] = \frac{M \sigma_e^2}{2M_T^2 Z_f(t)} \left( \alpha t \pm \frac{\gamma}{\sigma_e^2} \right)^2 + M \frac{p_0^2}{2M_T^2} + \frac{\epsilon}{\pi},
\] (2.24)
so that there is a negative energy transfer \( E \left[ H_M^+ (x(t), t) \right] - E \left[ H_M^- (x(t), t) \right] \approx -\frac{M\alpha^2 \gamma}{4 M_T^2 Z_T^2 (t)} \uparrow 0 \) which decreases with time. This shows that the heatbath is absorbing energy generated by the main particle initially but this approaches zero depending on the size of the term \( \alpha = 1/\chi M_T^2 \). For large objects \( \gamma \approx 0 \) so then this heat loss for the main particle will be negligible. Since the total energy is conserved this argument suggests that the heatbath must be gaining energy as a function of time which indeed will be shown below. This is an example of a case where the total energy is conserved as demanded by the non-radiation condition but only because both component energies change in time. To conserve \( E \left[ H_T \right] \) is therefore not equivalent to demanding that the backward and forward energies for the main particle are equal.

The average energy for the main particle equals

\[
E \left[ H_{M,\text{avg}} (x(t), t) \right] = \frac{1}{2} E \left[ H_M^+ (x(t), t) + H_M^- (x(t), t) \right] = M\sigma_e^2 \left( \frac{\alpha^2 \gamma^2}{2M_T^2 Z_T^2 (t)} + \frac{\gamma^2}{\sigma_e^2} \right) + M\frac{p_0^2}{2M_T^2} + \frac{\epsilon}{\tau}.
\]

In the case that \( \alpha t \approx 0 \) - equivalent to a very short time step \( t \approx 0 \) or a very small mass ratio \( \gamma \approx 0 \) - the average main particle energy reduces to

\[
E \left[ H_{M,\text{avg}} (x(0), 0) \right] = \frac{1}{2} E \left[ H_M^+ (x(0), 0) + H_M^- (x(0), 0) \right] = \frac{M\gamma^2}{2M_T^2 Z_T^2 (t)} + M\frac{p_0^2}{2M_T^2} + \frac{\epsilon}{\tau}.
\]

On the other hand from (2.24) it is clear that

\[
E \left[ H_{M,\text{avg}} (x(\infty), \infty) \right] = \frac{1}{2} E \left[ H_M^+ (x(\infty), \infty) + H_M^- (x(\infty), \infty) \right] = \frac{M\sigma_e^2}{2M_T^2} + M\frac{p_0^2}{2M_T^2} + \frac{\epsilon}{\tau},
\]

since \( \frac{\gamma^2}{Z_T^2 (t)} \to 1 \). Notice that the terms \( M\sigma_e^2/(2 M_T^2) \) and \( M p_0^2/(2 M_T^2) \) in the limit energies \( E \left[ H_{M,\text{avg}} (x(\infty), \infty) \right] \) and \( E \left[ H_{M,\text{avg}} (x(0), 0) \right] \) are close in size to the first two terms in (2.24) as long as \( \gamma \) is small. However the diffusion term is (2.24) is very large in comparison to the diffusion term \( \epsilon/\tau \) in \( E \left[ H_{M,\text{avg}} (x(\infty), \infty) \right] \) and \( E \left[ H_{M,\text{avg}} (x(0), 0) \right] \) see the discussion below.

To investigate the heatbath apply Corollary (2.15) to determine that for the heatbath particle

\[
g^\pm (x, t) = \frac{1}{\chi M_T Z_T (t)} \left( x - \frac{p_0 t}{M_T} \right) \left( \alpha t \mp \frac{1}{\gamma \sigma_e^2} \right) + \frac{p_0}{M_T},
\]

so that

\[
E \left[ H_m^\pm (x(t), t) \right] = \frac{m \sigma_e^2}{4 M_T^2 Z_T^2 (t)} \left( \alpha t \mp \frac{1}{\gamma \sigma_e^2} \right)^2 + m\frac{p_0^2}{2M_T^2} + \frac{m \omega^2}{\tau},
\]
and
\[ E[\mathcal{H}_{m,\text{avg}}(x(t), t)] = \frac{1}{2} E[\mathcal{H}^+_{m}(x(t), t) + \mathcal{H}_{m}^-(x(t), t)] = \frac{m \sigma^2}{2M_T^2Z^2(t)} \left( \alpha^2 t^2 + \frac{1}{\gamma^2 \sigma^2_t} \right) + m \frac{p_0^2}{2M_T^2} + m \omega^2 \frac{\tau}{\gamma^2}. \]

Hence
\[ E[\mathcal{H}_{m,\text{avg}}(x(0), 0)] = \frac{1}{2} E[\mathcal{H}^+_{m}(x(0), 0) + \mathcal{H}_{m}^-(x(0), 0)] = \frac{M \sigma^2}{2M_T^2} + m \frac{p_0^2}{2M_T^2} + m \omega^2 \frac{\tau}{\gamma^2}, \quad (2.27a) \]

and for large time \( t \) the average heatbath energy becomes
\[ E[\mathcal{H}_{m,\text{avg}}(x(\infty), \infty)] = \frac{1}{2} E[\mathcal{H}^+_{m}(x(\infty), \infty) + \mathcal{H}_{m}^-(x(\infty), \infty)] = \frac{m \sigma^2}{2M_T^2} + m \frac{p_0^2}{2M_T^2} + m \omega^2 \frac{\tau}{\gamma^2}, \quad (2.27b) \]

which indeed decreases from \( M \sigma^2/(2M_T^2) \) to \( m \sigma^2/(2M_T^2) \) as time progresses.

It is interesting to compare the variance contributions to the energies \( \mathcal{H}_{m,\text{avg}} \), \( \mathcal{H}^+_{m} \) and \( \mathcal{H}^-_{m} \). Recall that \( m \omega^2/ \gamma^2 = m \sigma^2/(2\alpha^2) \). If \( \gamma \ll 1 \) then \( m \omega^2/ \gamma^2 >> \epsilon/\gamma^2 \) so the diffusion energy contribution to the heatbath particle is much larger than the diffusion energy for the main particle. The energy due to the dispersion term \( \sigma^2_t \) is at first a small contribution in the main particle energy in \( \mathcal{H}^+_{m} \) but then increases (see \( \mathcal{H}_{m,\text{avg}} \), \( \mathcal{H}^-_{m} \)) while this term in the heatbath particle energy \( \mathcal{H}^+_{m} \) does exactly the opposite (see \( \mathcal{H}_{m,\text{avg}} \), \( \mathcal{H}^-_{m} \)). Both the main and heatbath particle energy are proportional to the same kinetic energy contribution weighted with their respective masses. This implies that the kinetic energy is almost exclusively carried by the main particle and for small \( \gamma \) very little kinetic energy is carried by the heatbath particle. In fact in the small \( \gamma \) limit the heatbath particles are all moving through the heatbath with energy \( \mathcal{H}_{m,\text{avg}} \approx \sigma^2/(2\alpha^2) \approx \epsilon/(2\gamma^2) \) without being affected by the presence of the main particle. After the collision the heatbath particle emerges with exactly the same speed and opposite direction.

A curious consequence of this example seems to be that the statistical characteristics of the heatbath particles are affected by the energy constraint in a similar fashion as the main particle. The time dependent term in \( \mathcal{H}_{m,\text{avg}} \) shows a behavior that reflects the main particle and \( \mathcal{H}^-_{m} \) carries a kinetic contribution that is also present in \( \mathcal{H}^+_{m} \). This is slightly unrealistic as it seems to imply that the heatbath particle behavior depends additionally on the main particle kinetic energy rather than external factors alone. Though the effect becomes very small as the mass ratio \( \gamma \) decreases the only way to render equation \( \mathcal{H}^-_{m} \) time-independence is to assume that the average collision time \( \tau \) changes as a function of energy or correlate the drift dependence between pre- and post collision velocities. The next Section addresses these constructions.

### 3. The Minkowski Invariant

The example in the previous Section showed that a constant total kinetic energy can be achieved but the individual main and heatbath particles energies display time dependent behavior. This Section attempts to investigate the momentum constraint
to impose energy conservation embedded in the heatbath particles through the point of collision. It will be shown that the relationship between the inter-
particle collision time and the total energy leads to a type of geometric invariant.

To obtain an equation similar to (2.14) for the momentum constraint substitute (2.20) into (2.7b) to find

$$\frac{1}{2} \mu \left[ w_1^2 + w_2^2 \right] = \frac{1}{2} \mu \left[ \|w(t)\| \right]$$

$$= \frac{1}{2} \mu \left[ \frac{b^+(x(t), t) - b^-(x(t), t)}{2} \right]$$

(3.1)

where $b^+ = b^+(x(t), t)$ and $b^- = b^-(x(t), t)$ are the usual forward and backward drifts respectively, $\pi(x(t), t) = (b^+(x(t), t) + b^-(x(t), t)) / 2$ as defined in (2.13) and $\alpha = \gamma^4 / (1 + \gamma^4)$. Assuming that the underlying process is a martingale and applying equation (2.19) reduces this to

$$\frac{1}{2} \mu \left[ |w|_1^2 + |w|_2^2 \right] = \frac{1}{2} \mu \left[ \|w(t)\| \right]$$

$$= \frac{1}{2} \mu \left[ \frac{\sigma^2 \Delta x(t)}{\tau_2} \right]$$

(3.2)

The constant in this expression is the result of the fact that in one dimension

$$\frac{1}{4} \left( 1 + \frac{1}{\gamma^4} \right) \mu \left[ \left( \frac{\sigma^2 \Delta x(t)}{\tau_2} \right) \right] = \frac{1}{4} \left( 1 + \frac{1}{\gamma^4} \right) \mu \left[ \frac{\sigma^2}{\tau_2} \right]$$

$$= \frac{1}{2} \left( 1 + \frac{1}{\gamma^4} \right) \frac{\sigma^2}{\tau} = \frac{1}{2} \left( 1 + \frac{1}{\gamma^4} \right) \frac{\epsilon}{M\tau} = \frac{1}{2} \frac{\gamma^4}{1 + \gamma^4} \frac{\epsilon}{M\tau} = \frac{\epsilon}{2\alpha^2 M\tau}$$

and multiplying with $n$ for the multi-dimensional case yields the value for the constant in (2.12).

In a heatbath where the main particle is in equilibrium with the incident particles it should be expected that the post-collision energy for the heatbath particle is equal to the pre-collision when averaged over all paths and positions. Otherwise there will be an average heat loss or gain for the main particle. So if the main particle is in equilibrium it is expected that $E \left[ w_2^2 \right] = E \left[ w_2^2 \right] = c^2$ where $c$ is the average velocity of the heatbath particles. This means that $\frac{1}{2} \mu \left[ E \left[ w_2^2 \right] + E \left[ w_1^2 \right] \right] = c^2$ and defining $\Delta \pi_\tau$ as

$$\left| \Delta \pi_\tau \right|^2 = \frac{1}{2} \mu \left[ \left( \frac{\pi(x(t), t)}{\tau_2} \right) \right]$$

(3.3)

reduces equation (3.2) to

$$c^2 = \frac{\left| \Delta \pi_\tau \right|^2}{\tau^2} + \frac{\epsilon}{\alpha^2 M\tau}$$

Hence

$$\left| \Delta \pi_\tau \right|^2 = \frac{\left| \Delta \pi_\tau \right|^2}{\alpha^2 M\tau}$$

(3.4)

The results can now be summarized in the following theorem
Theorem 3.1. Let \( x(t) \in \mathbb{R}^n \) be the coordinate process of the main particle and define \( |\Delta \mathbf{x}|^2 \) as in equation (3.3). Assume that the main particle is not radiating energy or receiving energy so that the backward and forward velocities of the heatbath particle are equal, e.g. \( E[w_2^2] = E[w_1^2] = c^2 \). Then the drifts must be such that 
\[
c^2 \tau^2 - |\Delta \mathbf{x}|^2 \quad \text{forms an invariant of the motion, i.e.}
\]
\[
j = N \sum_{j=0}^{j=N} \left( c^2 \tau^2 - |\Delta \mathbf{x}|^2 \right) = \frac{n \epsilon T}{2 \alpha^2 M} = \text{constant},
\]
where \( N \) is the average number of collisions such that \( E\left[ \sum_{j=1}^{j=N} \tau_j \right] = N \bar{\tau} = T \).

Proof. The proof is simply that (3.4) implies that 
\[
j = N \sum_{j=0}^{j=N} \left( c^2 \tau^2 - |\Delta \mathbf{x}|^2 \right) = \frac{n \epsilon T}{2 \alpha^2 M},
\]

since \( N \) is the (average) number of inter-particle collisions between time 0 and time \( T \). The righthand side is independent of the average inter-particle collision time. □

Remark 3.2. If \( |\Delta \mathbf{x}|^2 \approx 0 \) and \( c^2 \) is large then the solution to equation (3.5) equals
\[
\bar{\tau} = \frac{n \epsilon}{2 c^2 \alpha^2 M},
\]
so there is a reference average inter-particle collision time for a slow-moving (stationary) main particle in the heatbath. Combining this and (3.5) shows immediately that
\[
j = N \sum_{j=0}^{j=N} \left( c^2 \tau^2 - |\Delta \mathbf{x}|^2 \right) = c^2 T \bar{\tau}.
\]

To gain some insight into this Minkowski type relativistic invariant consider the example of the Gaussian wave packet in the previous Section. From equations (2.22) it is clear that
\[
\frac{1}{2} \left( b^+ (x, t) + b^- (x, t) \right) = \frac{\alpha t}{\chi M T Z(t)} \left( x - \frac{p_0 t}{M T} \right) + \frac{p_0}{M T} \approx \frac{p_0}{M T},
\]
\[
\frac{1}{2} \left( b^+ (x, t) - b^- (x, t) \right) = \frac{\gamma}{\chi M T Z(t) \sigma^2} \left( x - \frac{p_0 t}{M T} \right) \approx 0,
\]

since \( \alpha t / Z(t) \approx 0 \) and \( 1 / Z(t) \approx 0 \) for sufficiently large time \( t \). As a result equation (3.5) becomes
\[
j = N \sum_{j=0}^{j=N} \left( c^2 \tau^2 - \left( \frac{p_0}{M T} \right)^2 \right) = c^2 T \bar{\tau}.
\]

This suggests that the average inter particle collision time \( \bar{\tau} \) depends on the mean motion of the main particle specifically \( \bar{\tau} \sim \left( c^2 - \left( \frac{p_0}{M T} \right)^2 \right)^{-1} \). However this suggests that the drift \( |\Delta \mathbf{x}| \) does not depend on the average inter-particle collision time \( \bar{\tau} = \bar{\tau} \left( |\Delta \mathbf{x}| \right) \) which is unlikely to be reasonable. In general the mean inter-collision time and the drift will depend on each other and the most straightforward approach is to explore a linear relationship.
There does not seem to be a separate mechanism for introducing a dependent inter-collision time such that (3.5) holds except possibly a statistical correlation between the forward and backward velocities $\Delta^+ z$ and $\Delta^- z$. This creates a separate relationship between the correlation $\text{corr} \left( \frac{\Delta^+ z}{\tau_2}, \frac{\Delta^- z}{\tau_1} \right) = \rho_{\Delta^+ z, \Delta^- z} I$ ($I$ being the unit matrix) of the coordinate process $x(t)$ and the inter-particle collision time $\tau$. Returning to (3.7) and introducing the correlation term shows that

$$c^2 = \frac{1}{2} E \left[ |v(x(t), t)|^2 \right]$$

$$+ \frac{1}{8\gamma^4} E \left[ |b^+(x(t), t) - b^-(x(t), t)|^2 \right]$$

$$+ \frac{\sigma^2}{8} \left( \frac{\Delta^+ z}{\tau_2} + \frac{\Delta^- z}{\tau_1} \right)^2 \right]$$

$$+ \frac{\sigma^2}{8\gamma^4} E \left[ \left( \frac{\Delta^+ z}{\tau_2} - \frac{\Delta^- z}{\tau_1} \right)^2 \right]$$

$$= \frac{\Delta^2\tau_v^2}{\tau^2} + \frac{n \epsilon}{\alpha^2 M \tau} + \left( 1 - \frac{1}{\gamma^2} \right) \frac{n \epsilon \rho_{\Delta^+ z \Delta^- z}}{2M \tau}$$

$$= \frac{\Delta^2\tau_v^2}{\tau^2} + \frac{n \epsilon}{2\alpha^2 M \tau} (1 - \rho_v^2),$$

if $\rho_v^2 = (1 - 2\alpha^2) \rho_{\Delta^+ z \Delta^- z}$. Multiplying with $\tau^2$ and dividing by $(1 - \rho_v^2)$ this can be written as

$$c^2 \tau_v^2 = |\Delta^2\tau_v^2| + \frac{n \epsilon \tau}{2\alpha^2 M},$$

where

$$\tau_v = \frac{\tau}{\sqrt{1 - \rho_v^2}},$$

$$|\Delta^2\tau_v| = \frac{1}{2} \left( \frac{E [\tau(x(t), t)|^2]}{\frac{v^2}{2}} + \frac{\epsilon}{\gamma^2} E \left[ \left| b^+(x(t), t) - b^-(x(t), t) \right|^2 \right] \right) \tau_v^2.$$ 

This means that (3.8) reduces to

$$\sum_{j=0}^{N_{\tau}} \left( c^2 \tau_v^2 - |\Delta^2\tau_v|^2 \right) = \frac{n \epsilon T}{2\alpha^2 M},$$

where now the summation ranges over $N_{\tau}$ rather than over $N_{\tau_v}$. To obtain an estimate of the size of the correlation assume that $\tau \approx \tau_0$, write $v^2 = |\Delta^2\tau_v|^2 / \tau_v^2$, then substitute (3.7) into (3.8) to yield

$$\sum_{j=0}^{N_{\tau}} \left( c^2 \tau_v^2 - |\Delta^2\tau_v|^2 \right) = \frac{T}{\tau_0} \left( c^2 \tau_v^2 - v^2 \tau_v^2 \right) = \frac{n \epsilon T}{2\alpha^2 M} = c^2 \tau_0 T,$$

which is equivalent to

$$\frac{\tau_v^2}{\tau_0^2} = \frac{1}{1 - \frac{v^2}{c^2}}.$$

As a result then equation (3.7) shows immediately that $\rho_v^2 \approx v^2/c^2$.

Interpreting $\tau$ and $|\Delta^2\tau_v|^2$ as differentials equation (3.7) becomes the well known Minkowski invariant in Relativity Theory and its solution is the (linear) Lorentz
transformation which relates elapsed time versus motion as perceived in different reference frames. The following Theorem summarizes the results and shows the simple linear transformation.

**Theorem 3.3.** Let the main particle in the heatbath be in energetic equilibrium with the heatbath so that \( E \left[ w_z^2 \right] = E \left[ w_T^2 \right] = c^2 \) at any collision point \( t \). Now let the forward and backward velocities \( \Delta^+ z \) and \( \Delta^- z \) be statistically correlated so that \( \text{corr} \left( \Delta^+ z / \tau_1, \Delta^- z / \tau_1 \right) = \rho_{\Delta^+ z, \Delta^- z} \) and let \( \rho^2 = \left( 1 - 2\alpha^2 \right) \rho_{\Delta^+ z \Delta^- z} \). Then condition (3.1) is equivalent to

\[
\sum_{j=0}^{nT} (\Delta^2 \tau_v | - | \Delta^2 \tau_v |) = \frac{nT}{2\alpha^2 M}, \tag{3.10}
\]

where \( nT = T/\tau \) is the average number of collisions in time \( T \) assuming inter-collision time \( \tau \) and where

\[
\tau_v = \frac{\tau}{\sqrt{1 - \rho^2}}.
\]

\[
|\Delta^2 \tau_v |^2 = \frac{1}{2} \left( \frac{E \left[ v^2 (x(t), t) \right]}{\rho^2} \right) \Delta^2 \tau_v.
\]

Now if \( v = \Delta^2 \tau_v / \tau_v \) and \( v' = \Delta^2 \tau / \tau \) the solution to equation (3.10) equals

\[
\left( \Delta^2 \tau_v / \tau_v \right) = \frac{1}{1 - \frac{v - v'}{c^2}} \left( \frac{1}{\rho^2} \right) \left( \frac{(v - v')^T}{c^2} \right) \left( \frac{(\Delta^2 \tau_v / \tau) \Delta^2 \tau / \tau} {1} \right). \tag{3.11}
\]

**Proof.** For the more formal solution to (3.10) let \( \Delta \tau_v \) be the drift associated with the inter-collision time \( \tau \) and \( \Delta \tau_v \) be the (larger) drift associated with the inter-collision time \( \tau_v \) then the invariance condition (3.10) suggests that

\[
\left( \begin{array}{c}
\Delta \tau_v \\
\tau_v
\end{array} \right) = \left( \begin{array}{cc}
A & B \\
F & E
\end{array} \right) \left( \begin{array}{c}
\Delta \tau_v \\
\tau_v
\end{array} \right) = \left( \begin{array}{c}
A \Delta \tau_v + B \tau_v \\
F \Delta \tau_v + E \tau_v
\end{array} \right) \tag{3.12}
\]

for a constant matrix \( A \in \mathbb{R}^{n \times n} \), \( B, F^T \in \mathbb{R}^{n \times 1} \) and \( E \) a constant. Substituting this into (3.10) yields

\[
c^2 \tau_v^2 - |\Delta \tau_v |^2 = c^2 \left( E \tau + F \Delta \tau_v \right)^2 - |A \Delta \tau_v + B \tau_v|^2
\]

\[
= \left( c^2 E^2 - |B|^2 \right) \tau_v^2 - \Delta \tau_v^T \left( A^T A - c^2 F^T F \right) \Delta \tau_v, \tag{3.13}
\]

where \( c^2 E F^T = AB \) is chosen to avoid mixing terms. Applying \( \tau = \tau_0 \) then \( \Delta \tau_{\tau_0} = 0 \) so that (3.13) reduces to

\[
\left( \begin{array}{c}
\Delta \tau_v \\
\tau_v
\end{array} \right) = \left( \frac{\Delta \tau_v}{\tau_v} \right),
\]

and define \( B/E = v = \Delta \tau_v / \tau_v \in \mathbb{R}^n \).

From \( c^2 E F^T = AB \) it then follows that \( F^T = Av/c^2 \). Equation (3.13) now reduces to

\[
c^2 \tau_v^2 - \Delta \tau_v^2 = E^2 \left( 1 - \frac{|v|^2}{c^2} \right) c^2 \tau_v^2
\]

\[
- \Delta \tau_v^T \left( A^T A - c^2 v^T F^T F v \right) \Delta \tau_v \tag{3.14}
\]
Applying this to the $\tau_0, \Delta \tau \approx 0$ case shows that $E = 1/\sqrt{1 - \frac{v^2}{c^2}}$, so that finally
$$c^2 \tau_0^2 - |\Delta \tau_0|^2 = E^2 \left(1 - \frac{v^2}{c^2}\right) c^2 \tau^2 = c^2 \tau^2.$$ 

Hence equation (3.12) applies to the drift/time pair $\Delta \tau_0, \tau_0$ and $\Delta \tau_0 \approx 0, \tau_0$ hence
$$\left(\Delta \tau_0 \tau_0\right) = \left(A(v) B(v) E(v) F(v)\right) \left(\Delta \tau_0 \tau_0\right).$$

Moreover equation (3.12) relates the drift/time pair $\Delta \tau, \tau$ and $\Delta \tau_0 \approx 0, \tau_0$ so again
$$\left(\Delta \tau \tau\right) = \left(A(v') B(v') E(v') F(v')\right) \left(\Delta \tau \tau\right).$$

Finally from these two equations it is clear that
$$\left(\Delta \tau_0 \tau_0\right) = \left(A(v) B(v) E(v) F(v)\right) \left(\Delta \tau_0 \tau_0\right) = \left(A(v') B(v') E(v') F(v')\right) \left(\Delta \tau \tau\right),$$

which yields (3.11) so the argument is complete. \hfill $\Box$

Remark 3.4. The analogy with relativity extends further than just the Lorentz transformation above. For example, for the kinetic energy of the main particle it is possible to write $E[\mathcal{H}_T] \approx \frac{1}{2} M v^2 \approx \frac{1}{2} M v^2$, ignoring the osmotic term, the effect of a finite mass ratio and the diffusion term in (2.15). Expressing the differential $|\Delta \tau_0|^2$ in terms of $\tau_0$
$$E[\mathcal{H}_k] \approx M |\Delta \tau_0|^2 \tau_0^2 = M \left(c^2 - \frac{mc}{2\tau_0 a^2 M}\right)$$
$$= Mc^2 \left(1 - \frac{\tau_0}{\tau_0}\right) = Mc^2 \left(1 - \sqrt{1 - \frac{v^2}{c^2}}\right),$$

and recalling the definition of the relativistic energy $E_r = Mc^2/\sqrt{1 - v^2/c^2}$, this equation can be rewritten as
$$\frac{M}{\sqrt{1 - \frac{v^2}{c^2}}} \frac{|\Delta \tau_0|^2 \tau_0^2}{\tau_0^2} = \frac{Mc^2}{\sqrt{1 - \frac{v^2}{c^2}}} - Mc^2 = E_r - Mc^2,$$

which yields
$$E_r = M_r |\Delta \tau_0|^2 \tau_0^2 + Mc^2 = \frac{E[\mathcal{H}_k]}{\sqrt{1 - \frac{v^2}{c^2}}} + Mc^2,$$ (3.15)

with $M_r = \frac{M}{\sqrt{1 - \frac{v^2}{c^2}}}$ the relativistic mass.
The remark allows an interesting interpretation of the various terms $E[H_k]$, $c$ and the diffusion term $\epsilon/(\alpha^2 M^\tau)$. Clearly the relativistic mass $M$ in this context is the mass measured as a function of correlation while the kinetic energy $E[H_k]$ refers to the total kinetic energy of the associated main particle and is in Relativity Theory referred to as the relativistic momentum. The second term on the righthand side of (3.15) is the rest energy of the main particle and is in the present context the result of the diffusion energy. In fact, using (3.6) it is clear that

$$Mc^2 = \frac{ne}{2a^2\tau_0},$$

interpreting the relativistic mass in terms of the mass ratio $\gamma$, the average intercollision time $\tau_0$ for the main particle at rest in the heatbath and the variance per mass ratio $\epsilon$ (with units of action).

The most important conclusion from these observation is that it is possible to find a simple relationship between the inter-particle collision time and forward/backward (main) particle velocity correlation in the form of the Lorentz transformation, see Lanczos [17] for some more detail. The relativity analogy can be pushed further and the relativistic momentum and the rest mass energy of the main particle can be interpreted in terms of the time to collision, mass ratio and variance per unit mass $\epsilon$. Unfortunately, the compounded correlation $\rho^2 = (1 + 2\alpha^2) \rho_{\Delta^+ z \Delta^- z}$ destroys the martingale property for the coordinate process of the main particle and this in turn affects the correlation structure of the heatbath particle. Theorem 2.8 shows the heatbath backward and forward velocity are correlated already so the superimposed correlation will have an additional effect as shown below.

The remaining part of this Section will briefly discourse on a correlation model for the impulses $\frac{1}{\tau_1} \sigma^a \Delta^+ z$ and $\frac{1}{\tau_1} \sigma^a \Delta^- z$. A convenient route is to assume that

$$\begin{pmatrix} \sigma_{\Delta^+ z} \\ \sigma_{\Delta^- z} \end{pmatrix} = \begin{pmatrix} \sigma_a \Delta_a \\ \sigma_a \Delta_a \end{pmatrix} + \begin{pmatrix} \sigma_a \Delta_a \\ -\sigma_a \Delta_a \end{pmatrix} + \begin{pmatrix} \sigma_o \Delta^+ \Delta^- \\ \sigma_o \Delta^+ \Delta^- \end{pmatrix}, \tag{3.16}$$

where $\Delta^+ z$, $\Delta^- z$ are independent Gaussian increments, $\sigma_a = \sigma_a(x,t)$, $\sigma_o = \sigma_o(x,t)$ are $n \times n$ matrices and $\Delta_a \in \mathbb{R}^n$ and $\Delta_a \in \mathbb{R}^n$ independent processes with $E[\Delta_a \Delta^T_a] = E[\Delta_a \Delta^T_a] = 2I$. Proper conditions on the drift and variance terms will not be specified here. This representation is motivated by the fact that by this construction $\Delta^+ x(t,\beta) - \Delta^- x(t,\beta)$ does not depend on $\sigma_o \Delta_a$ and $\Delta^+ x(t,\beta) + \Delta^- x(t,\beta)$ becomes independent of $\sigma_o \Delta_a$.

The form of the correlation can now be summarized in a straightforward calculation as follows.

**Proposition 3.5.** If the correlation structure of the main particle is represented by equation (3.16) then the random variables $\Delta_a$ and $\Delta_a$ are part of both the past and the future steps of the process or rather relate the past to the future. The correlation
structure of the heatbath particle is then represented by
\[
\begin{pmatrix}
\frac{\Delta^+}{\tau_2} \\
\frac{\Delta^-}{\tau_1}
\end{pmatrix} = \frac{1}{\gamma \sin(\theta)} \begin{pmatrix}
-\cos(\theta) & 1 \\
1 & -\cos(\theta)
\end{pmatrix} \begin{pmatrix}
\sigma_a \Delta^+ \\
\sigma_a \Delta^-
\end{pmatrix} + \sigma_a \Delta_o \begin{pmatrix}
1 \\
1
\end{pmatrix} - \sigma_o \Delta_o \begin{pmatrix}
1 \\
1
\end{pmatrix} \frac{1}{\gamma^2} \begin{pmatrix}
-\cos(\theta) & 1 \\
1 & -\cos(\theta)
\end{pmatrix} \begin{pmatrix}
\Delta^+ \\
\Delta^-
\end{pmatrix}
\]
(3.17)

where \(\Delta^+, \Delta^-, \sigma_a(x, t), \sigma_o(x, t), \Delta_o \in \mathbb{R}^n\) and \(\Delta_a \in \mathbb{R}^n\) are defined above.

Proof. The first remark in the proposition is seen from the fact that equation (3.16) implies that
\[
2\sigma_a \Delta_o = \frac{1}{\gamma \sin(\theta)} \begin{pmatrix}
-\cos(\theta) & 1 \\
1 & -\cos(\theta)
\end{pmatrix} \begin{pmatrix}
\sigma_a \Delta^+ \\
\sigma_a \Delta^-
\end{pmatrix}
\]
(3.18)

The matrix in the proposition is the result of inverting equation (3.16) so (3.17) follows from the fact that the \(\Delta_a \in \mathbb{R}^n\) and \(\Delta_o \in \mathbb{R}^n\) terms are eigenvectors. In fact,
\[
\frac{1}{\gamma \sin(\theta)} \begin{pmatrix}
-\cos(\theta) & 1 \\
1 & -\cos(\theta)
\end{pmatrix} \begin{pmatrix}
\sigma_a \Delta^+ \\
\sigma_a \Delta^-
\end{pmatrix} = \begin{pmatrix}
\sigma_a \Delta_o \\
\sigma_a \Delta_o
\end{pmatrix},
\]
\[
\frac{1}{\gamma \sin(\theta)} \begin{pmatrix}
-\cos(\theta) & 1 \\
1 & -\cos(\theta)
\end{pmatrix} \begin{pmatrix}
\sigma_o \Delta^+ \\
\sigma_o \Delta^-
\end{pmatrix} = -\frac{1}{\gamma^2} \begin{pmatrix}
\sigma_o \Delta_o \\
\sigma_o \Delta_o
\end{pmatrix},
\]
since \(\frac{1-\cos(\theta)}{\gamma \sin(\theta)} = 1\) and \(\frac{1+\cos(\theta)}{\gamma \sin(\theta)} = 1/\gamma^2\). This completes the Proposition. \(\Box\)

To show the effect of the \(\sigma_a \Delta_o\) and \(\sigma_o \Delta_a\) terms take for example \(n = 1\), then equating the variances on both sides of (3.16)
\[
2\sigma^2 = \sigma^2 + \sigma_o^2 + \sigma^2 + \frac{2\sigma^2}{\gamma^2}.
\]
(3.19)

Since \(\Delta_a\) and \(\Delta_o\) are independent \(\sigma^2 E\left[\frac{\Delta^+ \Delta^-}{\tau_2 \tau_1}\right] = \sigma_o^2 var(\Delta_a) - \sigma_o^2 var(\Delta_o)\) so that the correlation between between \(\Delta^+ z\) and \(\Delta^+ z\) reduces to
\[
\rho_{\Delta^+ z \Delta^- z} = \frac{\sigma_o^2 var(\Delta_a) - \sigma_o^2 var(\Delta_o)}{\sigma^2 var(\Delta_a) + \sigma^2 var(\Delta_o) + \frac{2\sigma^2}{\gamma^2}}.
\]
(3.20)

If it is assumed that \(var(\Delta_a) = 2/\gamma = var(\Delta_o) = 2/\gamma\) then (3.20) reduces further to
\[
\rho_{\Delta^+ z \Delta^- z} = \frac{\sigma_o^2 - \sigma_o^2}{\sigma^2 + \sigma^2 + \frac{2\sigma^2}{\gamma^2}}.
\]
(3.21)

The reason for this construction now becomes clear. If \(\sigma_a \approx 0\) and \(\sigma_o >> \sigma_r\) then \(\rho_{\Delta^+ z \Delta^- z} \rightarrow -1\) while \(\rho_{\Delta^+ z \Delta^- z} \rightarrow 1\) if \(\sigma_o \approx 0\) and \(\sigma_a >> \sigma_r\). The correlation in the driving factors in (3.16) relates the future to the past through the collision time \(t\). This introduces a form of auto-correlation for the random difference process. For a
positive or negative correlation the process \( x(t, \beta), t > 0 \) can not be a martingale and a two dimensional process must be introduced.

This Section relates correlation in the motion of the main particle to the inter-particle collision time via the Lorentz equation to satisfy a Minkowski invariant and suggest that the rest mass energy is the result of the energy embedded in the diffusion energy. Proposition (3.5) shows how to decompose the backward and forward velocities into a perfect correlation part and a martingale process. These results were predicated on the interaction prescription (2.6) which is exact in the one-dimensional case. In higher dimensions the equation applies to the center of mass line projection as remark (2.4) describes. The energy conservation arguments in the last two Sections still apply however another level of complexity will be required to describe the non-simple collision. This will be addressed in the following Section.

4. Non-Simple Collisions / Scattering

This Section returns to the case where the matrix \( \Omega \) in equation (2.6) characterizes all elastic interactions incorporating the random anti-symmetric matrix \( Z = Z(U) \). In this case the total energy defined in Theorem (2.5) depends on the statistical characteristics of \( Z \) and Proposition (2.10) is derived in the presence of this collision scattering matrix. Finally the conservation condition for the full collision is derived and an example is presented that combines this result with an electromagnetic field type Hamiltonian. The Section concludes with showing that it is possible to subsume the collision scattering matrix \( Z \) into the heatbath making all the results from Section 2 and 3 applicable for an altered heatbath with a different statistical structure.

The first step is to obtain the total kinetic energy expression in Theorem (2.5) as a function of the pre- and post collision velocities \( v_2, v_1 \) of the main particle using equations (2.2) and (2.5). The form of the total kinetic energy is introduced in the following result.

**Theorem 4.1.** As in Theorem (2.5), let the momentum of the main particle and interacting particle be presented as \( p_1 = Mv_1 \) (post-collision \( p_2 = Mv_2 \)) where \( p_1, p_2, v_1, v_2 \in \mathbb{R}^n \) and \( q_1 = Mw_1 \) (post-collision \( q_2 = Mw_2 \)) with \( q_1, q_2, w_1, w_2 \in \mathbb{R}^n \). Then the total kinetic energy \( H_k = \frac{1}{2}(M|v_2|^2 + m|w_2|^2) = \frac{1}{2}(M|v_1|^2 + m|w_1|^2) \) is related to the pre- and post collision momenta of the main particle as follows

\[
\frac{8H_k}{MT} = \Delta^+ v^T \Delta^+ v - 2\Delta^+ v^T Z \Delta^- v \\
+ \frac{1}{\gamma^2} \Delta^- v^T \Delta^- v + \left( \frac{1 + \gamma^2}{\gamma^2} \right) \Delta^- v^T ZZ^T \Delta^- v \\
= (\Delta^+ v - Z \Delta^- v)^T (\Delta^+ v - Z \Delta^- v) \\
+ \frac{1}{\gamma^2} \Delta^- v^T \Delta^- v + \frac{1}{\gamma^2} \Delta^- v^T ZZ^T \Delta^- v,
\]

(4.1)

where

\[
\Delta^+ v = v_2 + v_1, \\
\Delta^- v = v_2 - v_1.
\]

(4.2)
Here $Z = Z(U)$ is the anti-symmetric matrix ($Z^T + Z = 0$) such that $Z = I - 2 (I + U)^{-1} = I - \gamma \sin(\theta) Q^{-1}$ where the unitary matrix $U$ and $Q$ are defined in equation (2.4) above.

Proof. The proof can be found in Appendix B as well. □

As mentioned above the random collision scattering matrix $Z = Z(U)$ represents the collection of all possible elastic collision transitions and therefore contains the center of mass line information and the angle of impact between $v_1$ and $w_1$. The matrix will be different from one collision to the next and has a statistical mean $E[Z] = Z$ and variance $E[ZZ^T]$ which may be a function of the collision position $x(t)$. To deduce the expectation of the energy term $H_k$ use again (1.3) with the definition (4.1) to derive

$$\frac{8E[H_k]}{MT} = E(\Delta^T v^T \Delta v) - 2E(\Delta^T v^T Z \Delta \Delta v)$$

$$+ \frac{1}{\gamma^2} E(\Delta^T v^T \Delta v) + \left(\frac{1 + \gamma^2}{\gamma^2}\right) E(\Delta^T v^T ZZ^T \Delta v)$$

$$= E(\Delta^T v^T \Delta v) - 2E(\Delta^T v^T Z \Delta \Delta v)$$

$$+ \frac{1}{\gamma^2} E(\Delta^T v^T \Gamma \Delta v),$$

where $E[Z] = Z$ and $\Gamma = I + (1 + \gamma^2) E(ZZ^T)$. This is the result of taking the expectations over the random matrix $Z$ first and then rearranging the expression.

Alternatively, this expression can be written as

$$\frac{8E[H_k]}{MT} = E \left((\Delta^T v - Z \Delta v)^T (\Delta^T v - Z \Delta v)\right)$$

$$+ \frac{1}{\gamma^2} E \left(\Delta^T v^T (\Gamma - \gamma^2 ZZ^T) \Delta v\right).$$

Notice that the matrix in the last terms is positive definite since $\Gamma - \gamma^2 ZZ^T = I + ZZ^T + \gamma^2(2ZZ^T - \gamma^2 ZZ^T) = I + ZZ^T + \gamma^2 \text{var}(ZZ^T)$ with the obvious definition for $\text{var}(ZZ^T) = E[ZZ^T] - E[Z]E[Z]^T \geq 0$.

Again it is assumed that the change in expected energy equals the change of an appropriate potential $\Phi_p$ so that $\frac{d}{dt} E[H_T] = \frac{d}{dt} E[H_k + \Phi_p] = 0$. The following Proposition shows the form of the total energy (4.3) as a function of the backward and forward velocity.

**Proposition 4.2.** Reducing the expectations in (1.3) the total energy in can be expressed as

$$\frac{E[H_k] + E[\Phi_p]}{MT} = \frac{1}{2} E \left(\frac{P^T \varphi}{2} - 2 \frac{P^T \varphi \Gamma \varphi}{2} \right)$$

$$+ \frac{n \sigma^2}{2 \gamma} + \frac{\sigma^2}{2 \gamma^2} E[Tr(\Gamma)] + \frac{1}{MT} E[\Phi_p].$$

Proof. This expression can be easily derived from substituting (1.2) into (1.3). Let $z_1 = \left(\frac{\Delta^+}{\gamma^2} + \frac{\Delta^-}{\gamma^2}\right)$ and let $z_2 = \left(\frac{\Delta^+}{\gamma^2} - \frac{\Delta^-}{\gamma^2}\right)$ then $z_1$ and $z_2$ are independent and
is conserved if\[4.4\]

Moreover, it is easy to see that \(E\) linearly related via equation (2.2) for the matrices \(P,Q,V\) as in equation (4.4).

...with \(\bar{\delta}\) and forward drifts normally distributed. Hence
\[\text{Theorem 4.3.}\]

Now the equivalent of Theorem (2.12) is introduced to show the conditions for maintaining a constant total energy.

**Theorem 4.3.** Let \(\rho = e^{\frac{2\lambda b}{\sigma^2}} = e^{\frac{2\lambda b}{\sigma^2}}\) and introduce the sufficiently smooth functions \(A = A(x,t), S = S(x,t), x \in \mathbb{R}^n\) and constants \(\delta, \xi\) to express the backward and forward drifts \(b^+ = b^+(x,t), b^- = b^-(x,t), x \in \mathbb{R}^n, t > 0\) as follows
\[b^+ = \xi (\nabla S - A) + \gamma \delta \nabla R,\]
\[b^- = \xi (\nabla S - A) - \gamma \delta \nabla R.\]

Assume that the potential \(\Phi_{p}\) satisfies the following property
\[\frac{d}{dt} E[\Phi_p] = E\left[ (\nabla S - A) \cdot (\nabla \phi + \xi \hat{A}) \right]\]
\[= E\left[ (S_{x,j} - A_j) (\phi_{x,j} + \xi \hat{A}_j) \right],\]  
(4.5)

with \(\hat{A} = \frac{\partial A}{\partial t}\) using Einstein’s notation of summing all like indices. Let \(\mathcal{H}_k\) be defined as in equation (4.1) with \(Z\) a random matrix such that \(\Gamma^S = I + (\gamma^2)E[Z^T Z]\) and \(E[Z] = Z\). Then the total energy \(\mathcal{H}_T = \mathcal{H}_k + \Phi_p\) for the potential in \(\Phi_p\) in (4.4) is conserved if
\[\frac{d}{dt} \left( \frac{E[\mathcal{H}_k] + E[\Phi_p]}{M_T} \right) \]
\[= \frac{d}{dt} \frac{1}{2} E\left[ \frac{\xi^2 (\nabla S - A)^2}{\sigma^2} - 2\xi \delta \gamma (\nabla S - A)^T \nabla R \right] + \frac{d}{dt} \frac{1}{M_T} E[\Phi_p] \]
\[= \xi \int \rho \left( (S_{x,x} - A_p) \left( \xi S_{x} + \frac{\xi^2}{\sigma^2} (S_{x,x} - A_j) (S_{x,x} - A_j) \right) \right) \]  
\[\frac{\delta^2}{2} R_{x,j} \Gamma_{x,j}^2 R_{x,k} - \frac{\gamma^2}{2} (R_{x,j} \Gamma_{x,j}^2)_{x,k} \right) dx \]  
(4.6)

\[\int \rho \left( (S_{x,x} - A_p) \left( \xi - \frac{1}{M_T} \right) \right) A_p dx + \Xi(Z) \]
\[+ \frac{\sigma^2}{2 \gamma^2} \frac{d}{dt} E[Tr(\Gamma^S)] = 0,\]
where

$$\Xi(Z) = \frac{\xi}{2} \int \rho \left( \delta^2 R_{x_j} \Gamma_{jk} \right) dx$$

$$+ \frac{\eta \xi}{2 \delta} \int \rho \left( (\delta \gamma (S_{x_j} - A_j) \mathbf{Z}_{jk})_{x_k}x_p \right) dx$$

$$- \xi \delta \gamma \int \rho \left( (S_{x_jt} - A_j) \mathbf{Z}_{jk}R_{x_k} + (S_{x_j} - A_j) \mathbf{Z}_{jk}R_{x_k} \right) dx,$$

and where \(\text{Tr}(\Gamma^z)\) denotes the Trace of the matrix \(\Gamma^z\). Here

$$\dot{Z} = \frac{d}{dt} E[Z],$$

$$\dot{\Gamma}^z = \frac{d}{dt} E[ZZ^T].$$

**Proof.** For a proof consult Appendix C.

This representation exhibits three sizeable problems finding solutions for the time invariance of (4.4). First of all there is the fact that potentials \(\Phi_p = \Phi_p(x, t)\) do not typically admit property like (4.5) as the time derivative of the potential introduces terms like \(E \left[ \frac{\partial \Phi_p}{\partial t} \right] \). Obviously time independent potentials satisfy property (4.5) and as can be seen below Maxwellian type fields have this property as well. In fact if the \(Z\) term can be ignored for a moment then the following can be shown.

**Theorem 4.4.** Assume that \(Z \equiv 0\) and let \(\psi = \psi(x, t) = e^{R(x,t) + iS(x,t)}\), with \(\rho(x, t) = |\psi(x, t)|^2\) where

$$b^+ = \xi (\nabla S - A) + \gamma \delta \nabla R,$$

$$b^- = \xi (\nabla S - A) - \gamma \delta \nabla R,$$

and let \(E\) and \(B\) satisfy the (magnetically sourceless) Maxwell equations

$$\nabla \cdot E = \rho(x, t),$$

$$\nabla \times B - \xi \frac{\partial}{\partial t} E = \xi \left( \frac{b^+ + b^-}{2} \right) \rho(x, t),$$

$$\nabla \cdot B = 0,$$

$$\nabla \times E + \xi \frac{\partial}{\partial t} B = 0,$$

so that \(E = -\nabla \phi - \xi \frac{\partial}{\partial t} A\) and \(B = \nabla \times A\). Assume that \(\Phi_p = |E|^2 + |B|^2\) then

$$\frac{d}{dt} \left( E \frac{|H_k| + E|\Phi_p|}{M_T} \right) = 0,$$

if and only if

$$i \chi \psi = -\frac{1}{2M_T} (\chi \nabla - iA)^2 \psi + \phi(x, t) \psi,$$

with \(\chi = M_T \eta = M_T \sigma^2 / \gamma = \left( \gamma + \frac{1}{\gamma} \right) \epsilon\) and \(\delta = \xi = 1/M_T\).
Proof. The point of the proof is that for equations (4.8) it is true that
\[
\frac{d}{dt} E[\Phi_p] = \int \rho \left[ |E|^2 + |B|^2 \right] = -\int \rho \left[ \left( \frac{b_+ + b_-}{2} \right)^T E \right] = \int \rho \left[ \left( \frac{b_+ + b_-}{2} \right)^T \left( \nabla \phi + \xi A \right) \right].
\]
In other words the time change of the energy of the field in (4.8) sat isfies (4.5) and this is combined with proposition (C.1) and equation (C.5) from Appendix C. □

The second issue is the fact that the terms \( \delta \frac{2}{\gamma} \gamma S_j \Gamma R_{x_1} R_{x_1} +, k = 1, ..., n \) and \( \delta \frac{2}{\gamma} \gamma (R_j, \Gamma R_{x_1} R_{x_1}) \), \( k = 1, ..., n \) in Theorem (4.5) above depend on the random \( Z \) matrix which acts here as an arbitrary scaling factor. If the \( \Gamma \) matrix is diagonal is is possible to scale the solution derived for the case where \( Z \) is state independent. In fact the example below shows that a simple scaling applied to the factors in the wave function allows for a solution.

4.1. The two-step Scattering Matrix. This example derives a solution to equation (4.6) by rescaling the wave function as follows. Assume that \( n = 2, \xi = \frac{1}{\gamma}, A \equiv \phi \equiv 0 \) and define the anti-symmetric matrices \( Z(\nu), Z(-\nu) \) as follows
\[
Z(\nu) = \begin{pmatrix} 0 & \nu \\ -\nu & 0 \end{pmatrix}, Z(-\nu) = \begin{pmatrix} \nu & -0 \\ -0 & \nu \end{pmatrix}.
\]
Now let the probabilities \( p(\nu) \) and \( p(-\nu) \) be such that
\[
E[Z] = Z = p(\nu)Z(\nu) + p(-\nu)Z(-\nu),
E[ZZ^T] = p(\nu)Z(\nu)Z^T(\nu) + p(-\nu)Z(-\nu)Z^T(-\nu) = \nu^2 I,
\]
so that \( \dot{\Gamma} = 0, Tr \left( \dot{\Gamma} \right) = 0 \) with \( Z \) state independent (not a function of \( x(t) \)). Then \( \Gamma = I \left( 1 + (1 + \gamma^2) \nu^2 \right) = I \sigma \nu^2 \) and the solution that preserves the energy equation (4.6) reduces to
\[
\frac{d}{dt} \left( \frac{E[H] + E[\Phi_p]}{M_T} \right) = \xi \int \rho \left( S_{x_p} \left( -\frac{\delta}{2} \nabla R|2 - \frac{\sigma \delta^2}{2} \nabla R|2 \right) - \frac{\sigma \delta}{2} \Delta_x R - \frac{\sigma \delta}{2} \Delta_x R \right) \right) dx \quad (4.10)
\]
because the second term in equation (4.6) vanishes
\[
\frac{\eta\xi}{2\nu} \int \rho S_{x_p} \left( (\xi \delta \gamma S_{x_j} Z_{jk})_{x_k} \right) dx,
\]
by the example below shows that a simple scaling applied to the factors in the wave function allows for a solution.
and so do the last two terms. Hence the solution to (4.9) is given by Proposition (C.3) below as

\[ i\chi_\nu \psi_t = -\frac{\chi_\nu^2}{2M_T} \Delta_x \psi + \phi(x, t)\psi, \]  

(4.11)

where \( \psi = \psi(x, t) = e^{\frac{iMR(x,t) \cdot x + (\mathbf{Z}(x,t))}{\delta}} \) with \( \chi_\nu = M_T\eta/\sigma_\nu \), \( \xi = 1/M_T \) and \( \delta = 1/(\sigma_\nu M_T) \). Proposition (4.10) in Appendix C has some more details on the derivation.

This highlights the second feature of equation (4.6) which is that the effective osmotic term typically scales up due to the variance of the random matrix \( \mathbf{Z} \). This scaling never disappears if \( E[ZZ^T] > 0 \) however equation (4.6) can still be reduced to the case of the simple collision in Theorem (2.12) as example (4.1) shows. There is no real quantum mechanical analogy to this except that some of the terms in equation (4.10) are similar to the terms in the Bopp-Haag Hamiltonian where the additional derivatives are introduced to incorporate spin states, see for instance Nelson [7].

The third question on equation (4.6) is the effect of the \( \mathbf{Z} \) terms. The example above shows that these terms disappear for the case where \( \mathbf{Z} \) does not depend on the coordinate system. This is entirely due to the fact that \( \mathbf{Z} \) is anti-symmetric and their contribution to equation (4.6) remain conveniently zero even if the matrix \( \mathbf{Z} \) depends on time \( t \). As the mean collision scattering matrix relates to the average center of mass line and average angle of collision this quantity is unlikely to be dependent on the collision coordinate \( x(t) \) so this assumption is not unreasonable.

Obviously the presence of the \( \mathbf{Z} \) matrix changes both the correlation between \( v_2 \) and \( v_1 \) and simultaneously affects the correlation structure of the heatbath. If for instance the main particle path is a martingale for \( \mathbf{Z} \equiv 0 \) then "turning on" the \( \mathbf{Z} \) will create a correlation. If the collision scattering matrix \( \mathbf{Z} > 0 \) and the main particle path is a martingale then the correlation structure of the heatbath must change from the case that \( \mathbf{Z} \equiv 0 \). The following Proposition generalizes Theorem (2.8) and calculates the correlation of the heatbath particles for the latter case.

**Proposition 4.5.** Assume that the backward and forward velocities of the main particle are uncorrelated. Then the correlation matrix for the colliding heatbath particle given a realization of the random matrix \( \mathbf{Z} \) looks like

\[
E\left[ \begin{pmatrix} \Delta^+ & \Delta^- \end{pmatrix} \begin{pmatrix} \Delta^+ & \Delta^- \end{pmatrix} \right] = \frac{\sigma^2}{\pi\alpha^2} \left( \frac{1}{1 - 2\alpha^2} - (1 - 2\alpha^2) \right) + \Gamma_Z,
\]

where

\[
\Gamma_Z = \frac{2\sigma^2}{\pi\gamma \sin^2(\theta)} \left( E[ZZ^T] \Omega^T E[ZZ^T] \right),
\]

and where

\[
\Omega = (1 - \cos(\theta)\mathbb{I}) \mathbf{Z} + E[ZZ^T].
\]

**Proof.** For a straightforward calculation see Appendix D.
Remark 4.6. Though Proposition (4.5) specifies how the heatbath particle field must behave to guarantee that the main particle moves in a Markovian fashion the distribution of $x(t)$ has now become complicated. Clearly the distribution for $v_2, w_2$ must be convolved with the distribution for $v_1, w_1$ and $Z = Z(U)$ and is therefore not readily calculated.

The final question in this Section is whether there is a "momentum term" version of Theorem (3.3) and whether the complexity of equation (4.6) can be reduced. Interestingly this can indeed be achieved in a straightforward manner but some changes in assumptions will be required. The approach is to absorb the scattering matrix $Z$ into the heatbath and then show that the results from Section 2 and 3 apply for the transformed heatbath.

To implement this approach the $Δ^+ v$ and $Δ^- v$ must be rewritten in a more convenient form. From the proof of Proposition (4.5) in Appendix D it becomes clear that

$$\begin{pmatrix} w_2 \\ w_1 \end{pmatrix} = \frac{1}{\gamma \sin(\theta)} \begin{pmatrix} -\cos(\theta)I - Z & I + Z \\ I - Z & -\cos(\theta)I + Z \end{pmatrix} \begin{pmatrix} v_2 \\ v_1 \end{pmatrix}. $$

This can be simplified by writing

$$\begin{pmatrix} w_2 \\ w_1 \end{pmatrix} = \begin{pmatrix} Vv_1 + Gw_1 \\ w_1 \end{pmatrix} = \begin{pmatrix} V & G \\ 0 & I \end{pmatrix} \begin{pmatrix} v_1 \\ w_1 \end{pmatrix}, $$

and then use equation (3.8) and (3.9) from the Appendix to obtain

$$\begin{pmatrix} w_2 \\ w_1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} V & G \\ I & (2Q^{-1} - I) \end{pmatrix} \begin{pmatrix} \Delta^+ v \\ \Delta^- v \end{pmatrix}, $$

hence with $V_T = (2Q^{-1} - I)$ this reduces to

$$\begin{pmatrix} w_2 \\ w_1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} V & G \\ I & V_T \end{pmatrix} \begin{pmatrix} \Delta^+ v \\ \Delta^- v \end{pmatrix} = \frac{1}{2} \begin{pmatrix} V + G & -V + GV_T \\ I & V_T \end{pmatrix} \begin{pmatrix} \Delta^+ v \\ \Delta^- v \end{pmatrix} = \frac{1}{2} \begin{pmatrix} I & V_T - \frac{\gamma^2}{2}I \\ I & \gamma^2 I \end{pmatrix} \begin{pmatrix} \Delta^+ v \\ \Delta^- v \end{pmatrix}.$$

Inverting this relation yields

$$\begin{pmatrix} \Delta^+ v \\ \Delta^- v \end{pmatrix} = 2 \begin{pmatrix} \frac{\gamma^2}{2}V_T & I - \frac{\gamma^2}{2}V_T \\ \frac{\gamma^2}{2}I & \frac{\gamma^2}{2}I \end{pmatrix} \begin{pmatrix} w_2 \\ w_1 \end{pmatrix};$$

which means

$$\Delta^+ v = 2w_1 + \gamma^2 V_T \Delta^- w, \quad \Delta^- v = -\gamma^2 \Delta^- w.$$ 

Now $\gamma^2 V_T = I - (1 + \gamma^2) Z$ so then

$$\Delta^+ v = \Delta^+ w - (1 + \gamma^2) Z \Delta^- w, \quad \Delta^- v = -\gamma^2 \Delta^- w,$$

(4.12)
which can also be written as
\[
\begin{align*}
\Delta^+ v &= \Delta^+ w + 2W, \quad (4.13a) \\
\Delta^- v &= -\gamma^2 \Delta^- w. \quad (4.13b)
\end{align*}
\]

Here \( mW \) is the additional momentum such that
\[
-\mathcal{W} = \frac{1+\gamma^2}{2} Z(w_2 - w_1) = \frac{1+\gamma^2}{2} Z\Delta^- w.
\]

From this the following two Theorems are easily shown.

**Theorem 4.7.** The additional momentum defined in equation (4.13a) above is perpendicular to the \( \Delta^- w \), in other words
\[
\begin{align*}
\Delta^+ v &= \Delta^+ w, \quad (4.14a) \\
\Delta^- v &= -\gamma^2 \Delta^- w. \quad (4.14b)
\end{align*}
\]

Let \( w_{\tau,1} = w_1 + \mathcal{W}, \ w_{\tau,2} = w_1 + \mathcal{W} \) and define \( \Delta^+ v = w_{\tau,2} - w_{\tau,1}, \ \Delta^- v = w_{\tau,2} - w_{\tau,1} = w_2 - w_1 \) then equation (4.13a) reduces to
\[
\begin{align*}
\Delta^+ v &= \Delta^+ w, \quad (4.14c) \\
\Delta^- v &= -\gamma^2 \Delta^- w. \quad (4.14d)
\end{align*}
\]

hence
\[
\frac{1}{2} E \left[ \left| \frac{\Delta^+ v}{2} \right|^2 + \frac{1}{\gamma^4} \left| \frac{\Delta^- v}{2} \right|^2 \right] = c_{\tau}^2, \quad (4.14e)
\]

where \( c_{\tau}^2 = E \left[ |w_{\tau,2}|^2 \right] = E \left[ |w_{\tau,1}|^2 \right]. \)

**Proof.** To prove assertion (4.14a) consider (4.13a) and multiply with (4.13b) so that
\[
\begin{align*}
\Delta^- v^T \Delta^+ v &= \Delta^- v^T (\Delta^+ w + 2W) \\
&= -\gamma^2 \Delta^- w^T \Delta^+ w - \gamma^2 \Delta^+ W^T, \\
\end{align*}
\]
or
\[
|v_2|^2 - |v_1|^2 + \gamma^2 |w_2|^2 - \gamma^2 |w_1|^2 = -\gamma^2 \Delta^- w^T W.
\]

However the left hand side equals \( |v_2|^2 + \gamma^2 |w_2|^2 - \left( |v_1|^2 + \gamma^2 |w_1|^2 \right) = \mathcal{H}_k/M - \mathcal{H}_k/M = 0 \) by energy conservation hence \( \text{\( \gamma^2 \Delta^- w^T W = 0 \) and (4.13a) is proved.} \)

Assertion (4.14b) now follows since
\[
\begin{align*}
E \left[ |w_1 + \mathcal{W}|^2 \right] - E \left[ |w_2 + \mathcal{W}|^2 \right] \\
= E \left[ |w_1|^2 \right] - E \left[ |w_2|^2 \right] + 2E \left[ (w_1 - w_2)^T W \right] \\
= -2E \left[ \Delta^- w^T W \right] = 0,
\end{align*}
\]
and equation (4.14c) follows directly from (4.14c) and (4.14d) since
\[
\Delta^+ v^T \Delta^+ v + \frac{1}{\gamma^4} \Delta^- v^T \Delta^- v \\
= \Delta^+ w^T \Delta^+ w + \Delta^- w^T \Delta^- w \\
= \frac{1}{2} \left( |w_2^\top|^2 + |w_1^\top|^2 \right)
\]
This concludes the proof. \(\square\)

In other words, the momentum constraint on the forward and backward drift \(b^+\) and \(b^-\) with \(Z \neq 0\) with the heatbath particles moving at average speed \(c\) can be transposed into the case where \(Z \equiv 0\) with the main particle in a heatbath where the particles move at average speed \(c_T\). Here again \(-mW = \frac{1+\gamma^2}{2} mZ(w_2 - w_1) = -\frac{1+\gamma^2}{2} mZ\Delta^- w\) is the additional momentum. Moreover, due to (4.14b) and (4.14e) the momentum conservation requirement for \(w_{\uparrow,1}\) and \(w_{\uparrow,2}\) as described in Theorem (3.3) is equivalent to a requirement on \(w_1\) and \(w_2\). The sole difference between the original and the transposed case is that the correlation between \(w_{\uparrow,1}\) and \(w_{\uparrow,2}\) is different from the correlation between \(w_1\) and \(w_2\) due to the fact that \(\mathcal{W}\) is a (random) function of \(w_1\) and \(w_2\). The exact expression is calculated in Proposition (4.5) for the case where the main particle follows a Markovian path. Any changes in correlation going from \(w_1, w_2\) to \(w_{\uparrow,1}, w_{\uparrow,2}\) suggest that the average inter-collision time is affected as detailed in Section 3.

The next result completes the identification between a heatbath \(w_2, w_1\) in which \(Z \neq 0\) and a heatbath \(w_{\uparrow,2}, w_{\uparrow,1}\) in which \(Z \equiv 0\). While (4.14e) is the transposed heatbath equivalent of the momentum constraint (2.7b) it is not immediately obvious that (2.7a) has an equivalent as well. The next Theorem shows that this is the case and as an addendum calculates the original energy in terms of the original heatbath terms.

**Theorem 4.8.** Let the main particle diffuse in a heatbath where \(w_{\uparrow,1} = w_1 + \mathcal{W}, w_{\uparrow,2} = w_2 + \mathcal{W}\) with \(-\mathcal{W} = \frac{1+\gamma^2}{2} Z(w_2 - w_1) = -\frac{1+\gamma^2}{2} Z\Delta^- w\). Then the total kinetic energy \(H_{\uparrow,k}\) equals
\[
\frac{8H_{\uparrow,k}}{M} = \Delta^+ v^T \Delta^+ v + \frac{1}{\gamma^4} \Delta^- v^T \Delta^- v \\
= \frac{1}{2} |v_1|^2 + \frac{1}{2} |w_{\uparrow,1}|^2 \\
= \frac{1}{2} |v_2|^2 + \frac{1}{2} |w_{\uparrow,2}|^2, \tag{4.15a}
\]
and
\[
\frac{8H_{\uparrow,k}}{M} = \Delta^+ v^T \Delta^+ v + \frac{1}{\gamma^4} \Delta^- v^T \Delta^- v \\
+ \gamma^2 \Delta^- w^T \Delta^+ w + \gamma^4 \Delta^- w^T \Delta^- w \\
= \frac{1}{2} |v_1|^2 + \frac{1}{2} |w_{\uparrow,1}|^2 \\
+ \frac{1}{2} \gamma^2 |v_2|^2 + \frac{1}{2} |w_{\uparrow,2}|^2 \\
+ \frac{1}{2} \gamma^4 |w_{\uparrow,2}|^2, \tag{4.15b}
\]

**Proof.** No calculations are required to show assertion (4.15a) as the definition of \(\mathcal{W}\) in (4.12) and (4.13a) shows that
\[
\begin{pmatrix} v_2 \\ v_1 \end{pmatrix} = \frac{\gamma}{\sin(\theta)} \begin{pmatrix} \cos(\theta) & 1 \\ 1 & \cos(\theta) \end{pmatrix} \begin{pmatrix} w_{\uparrow,2} \\ w_{\uparrow,1} \end{pmatrix}, \tag{4.16}
\]
using (D.3) and (D.4). From this it is easy to work back and derive
\[
(v_2, w_{\top,2}) = \begin{pmatrix} \cos(\theta) & \gamma \sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{pmatrix} (v_1, w_{\top,1}),
\]
which implies in turn that (2.7a) holds with \(w_{\top,1}, w_{\top,2}\) replacing \(w_1, w_2\). Hence
\[
\frac{H_{\top,k}}{M_T} = \frac{1}{2} \left| v_2 + v_1 \right|^2 + \frac{1}{2\gamma^2} \left| v_2 - v_1 \right|^2,
\]
with \(H_{\top,k} = \frac{M}{2} \left| v_1 \right|^2 + \frac{m}{2} \left| w_{\top,1} \right|^2 = \frac{M}{2} \left| v_2 \right|^2 + \frac{m}{2} \left| w_{\top,2} \right|^2\) but this is exactly assertion (4.15a).

Equation (4.15b) can be shown from straightforward calculation. Equation (B.13) shows that
\[
8 \frac{H_T}{M_T} - \Delta^+ w^T \Delta^+ w - \gamma^2 \Delta^- w^T \Delta^- w = -2 \Delta^+ w^T Z \Delta^- w + (1 + \gamma^2) \Delta^- w^T Z Z \Delta^- w,
\]
but from (4.12) it follows that
\[
\Delta^+ v^T \Delta^+ v + \frac{1}{\gamma^2} \Delta^- v^T \Delta^- v
\]
\[
= \Delta^+ w^T \Delta^+ w + \gamma^2 \Delta^- w^T \Delta^- w
\]
\[
+ (1 + \gamma^2) \left( -2 \Delta^+ w^T Z \Delta^- w + (1 + \gamma^2) \Delta^- w^T Z Z \Delta^+ w \right)
\]
\[
= \Delta^+ w^T \Delta^+ w + \gamma^2 \Delta^- w^T \Delta^- w
\]
\[
+ (1 + \gamma^2) \left( \frac{8 H_T}{M_T} - \Delta^+ w^T \Delta^+ w \right).
\]
Finally then
\[
\Delta^+ v^T \Delta^+ v + \frac{1}{\gamma^2} \Delta^- v^T \Delta^- v
\]
\[
= \frac{8 H_T}{M_T} - \gamma^2 \Delta^+ w^T \Delta^+ w
\]
\[
- \gamma^4 \Delta^- w^T \Delta^- w,
\]
which concludes the proof. □

5. Conclusions

The purpose of this paper is to revisit the classical diffusion problem of a main particle moving through a heatbath propelled by elastic collisions and introduce interaction energy and momentum considerations. The main particle path is modeled as moving linearly from one random collision to the next with random inter-collision times \(\tau_j, j \geq 0\), represented as second order Gamma distributions. This pre-limit microscopic construction models the motion of the main particle by collision positions \(x(t_j), j \geq 0\), at stopping times \(t_j, j \geq 0\), with \(t_{j+1} - t_j = \tau_j, j = 0, 1, \ldots\). The derived linear interpolated path \(x(t, \beta), t > 0\) constitutes a ”best estimate” of the main particle position. An important model assumption here is the choice of the second (or higher) order gamma distributions as the particle inter-collision times.
τ_j, j ≥ 0. If the distance traveled between the collisions x(t_j) and x(t_{j+1}) is modeled as b^+(x, t)τ_j and a (subordinate) Gaussian contribution then the inter-collision momentum and energy of the main particle is finite with probability one.

Section 1 shows that if the mean inter-collision times decreases the main particle path approaches the strong solution to the continuous stochastic differential equation with drift b^+(x, t). The drift and the variance term must satisfy standard requirements which guarantee the existence of a strong unique solution but one additional time growth condition on the drift was introduced to control the increasing multitude of "collision" path contributions. Some constraint must be applied to the time-variability of the drift because otherwise there is no guarantee that the drift specified at the collision points does not deviate too much from the continuous drift function.

Section 2 follows the consequences of the fact that the collisions with the heatbath particle are elastic and introduces the canonical solution to the collision energy and momentum conservation constraint. The pre- and post collision velocities of the colliding main and heatbath are linearly related via a matrix containing a random collision scattering matrix Z = Z(U) which carries the center of mass line and impact angle collision information. For simple collisions for which Z ≡ 0, U = I the canonical solution implies two constraints on the motion of the main particle. The first one relating the total kinetic energy (main and impacting heatbath particle combined) to the pre- and post-collision motion of the main particle. The second relationship has been referred to as the "momentum constraint" and looks more like a velocity requirement. If the total kinetic energy along the path of the main particle is not constant (on average) then some energy is being transferred between the main particle and the heatbath.

The main result in this Section shows that if there is no energy leakage (on average) between the main particle and the heatbath hence if the total kinetic energy plus possible potential is conserved then the probability distribution of the position of the main particle must be derived from Schrödinger’s equation. Planck’s constant is then replaced by a variance per unit of mass term ε and further depends on γ the mass ratio. The total energy functional may contain only certain suitable potentials satisfying an energy conservation property. The derivation relies heavily on the stochastic mechanics results and on convergence of the collision path representation to a suitable stochastic process.

The important aspect of this derivation is that a combined energy constraint for a particle diffusing through a heatbath is a purely classical problem and Schrödinger’s equation is invoked to prevent energy exchange between the main particle and the heatbath. The analogy with quantum mechanics however is not perfect as for instance the forward and backward drifts explode when the mass ratio γ becomes small. The present derivation moreover only allows certain appropriate potentials though this includes all time-independent potentials and the electromagnetic potentials see Section 2 and 4. Apart from the presence of the mass ratio γ there is an important conceptual difference. The total energy functional that is conserved by the presence of the Schrödinger wave function is the total kinetic energy of both the main and heatbath particle. Quantum mechanics associates the wave function only with the "main" particle and the energy eigenvalues of the wave function supposedly are the energy states of the main particle alone. In this paper the energy states obtained from the wave function relate to the combined main particle and
heatbath particle energy. Once the wave function solution has been obtained the main particle and heatbath particle energy contributions still need to be separated.

Yet another difference between the present formulation and the Theory of Quantum Mechanics is the curious aspect noted in the Gaussian Wave Packet example where the statistical characteristics of both the main and the heatbath particles are affected by the energy constraint. The kinetic and energy dispersion terms that are found in the energy of the main particle can also be found in the heatbath energies so the heatbath is affected by the presence of the main particle in a time dependent manner. This effect decreases if the mass ratio $\gamma$ becomes smaller but the model can not be structurally amended. The results in Section 3 suggest in fact that a different approach may be required which incorporates correlation between the main particle pre- and post collision velocities.

Intuition suggests that the diffusion/quantal effect becomes noticeable if the diffusion per mass term is significant in comparison to the size of the drift term or the energy dispersion. The example of the Gaussian Wave particle in Section 2 shows that the energy dispersion and the average main particle momentum increase the combined kinetic energy. This suggests that a high temperature heatbath environment that is not overly dense is dominated by its energy dispersion and mean particle drift. On the other hand if the main particle moves through a relatively narrow energy band with a relatively small kinetic motion then the diffusion term constitutes the larger part of the total kinetic energy. Ultimately if the heatbath is very dense then the diffusion term will become the dominant energy provider. A very dense heatbath environment eventually forces the dominant motion of the main particle to be entirely diffusive.

The example also shows that the heatbath looks like a reflection of the main particle. The main particle carries almost all the momentum and dispersion energy with little diffusion energy while the heatbath has a very large diffusion term and very little kinetic energy. If the pre- and post collision velocities of the main particle are uncorrelated as one would expect for a Markovian path then the pre- and post collision velocities for the heatbath particles will be correlated through the collision point. Both the main and heatbath particle kinetic energies are time dependent but the first one increases in size while the heatbath energy decreases proportionally. For a very small mass ratio $\gamma$ the time dependence almost disappears and the heatbath starts to behave as if it has only one velocity which is reflected by the collision.

The momentum constraint established in Section 2 shows that a similar symmetric quadratic expression employing the forward and backward velocities of the main particle can be directly related to the average velocity of the incident particle. The average is calculated as the arithmetic average of forward and backward heatbath particle velocity. The contribution of Section 3 is to show that if the heatbath particles are in energetic equilibrium with the main particle then the drift of the main particle and the correlation between the forward and backward velocities of the colliding heatbath particles must depend on the average inter-collision time. The condition is identical to the geometrical Minkowski invariant employed in Special Relativity and it is shown that the invariant can be satisfied by applying the Lorentz transformation to the average collision time and the squared distance traveled.
The analogy with Relativity Theory can be pushed further to suggest that the energy rest mass of the main particle equals its diffusive energy. In fact the rest mass can be expressed in terms of the mass ratio $\gamma$, the average inter-collision time $\tau_0$ for the main particle at rest in the bath and the variance per mass ratio $\epsilon$. This argument only employs the Lorentz transformation as a means of generating a solution to the Minkowski invariant and is not necessarily the only solution which balances the mean inter-collision time and the squared distance traveled. By comparison in Relativity Theory the homogeneity of space and the constancy of the speed of light in all directions leads to a unique solution.

The third set of results in section 4 focuses on the "non-simple" solution to the elastic collisions to include the random collision scattering matrix $Z$. The path of the main particle now becomes a "conditionally" Gaussian process in the sense that the main particle path process remains a Gaussian process given the realizations of the random collision scattering matrix $Z$. In general however the additional random matrix $Z$ alters the main particle coordinate distribution. The stochastic dynamics for the random matrix involve the center of mass line distribution and depend on the dimensions and physical setting rather than on the motion of the main particle. It is therefore reasonable to assume that the collision scattering matrix $Z$ does not depend on the pre- and post velocities of the main particle.

One of the most obvious effects of the random collision scattering matrix is the arbitrary change in correlation between the pre- and post collision bath velocities causing in turn a correlation between the pre- and post-collision velocity of the main particle. This destroys the Markovian property of the main particle path process so that additional variables must be introduced to model its motion. None of the results in Section 2 are then applicable because the fundamental Markovian result relating the backward and forward drift difference and main particle position probability density is not valid. However Section 3 demonstrates how the pre- and post-collision velocities correlation of the main particle process relates to the mean inter-particle collision time which can then be captured by the Lorentz transformation. Unfortunately there are no results that describe how the probability density of the main particle position can be calculated in the presence of correlation.

Theorem (4.3) in Section 4 presents the main result showing that the conservation of total energy depends on the mean scattering matrix $\overline{Z}$ and expected covariance matrix $E[ZZ^T]$. A full solution for the probability density has not been derived but for the case where $Z \equiv 0$ it was shown again that the probability density must be obtained employing Schrödinger’s equation as long as the potential is time independent or satisfies a Maxwell type set of equations. Another example is presented for the case where $Z$ is a function of time only while $E[ZZ^T]$ is a constant diagonal matrix. Then it is possible to obtain the probability for the main particle position in the form of a wave function for the $Z \equiv 0$ case but with some of the weighting parameters altered. In comparison to the $Z \equiv 0$ wave function this solution looks as if the mass weighting and the diffusion per unit of mass have changed to account for the collision scattering matrix.

A very useful result from this Section is that it is possible to absorb the collision scattering matrix $Z$ into the bath. Specifically it is possible to represent the case with a non-zero scattering matrix $Z \neq 0$ in a $w_1, w_2$ bath with the case where $Z \equiv 0$ with a $w_{1,1} = w_1 + W, w_{1,2} = w_2 + W$ bath. The additional momentum $mW$ is proportional to the collision scattering matrix $Z$ and acts as
a straight increase in the energy in the heatbath while it is orthogonal to the momentum exchange. However the correlation structure for $w_{\tau,1}, w_{\tau,2}$ is different from the correlation matrix for $w_1$ and $w_2$. Therefore the path for a diffusing main particle can not be Markovian in both the $w_1, w_2$ heatbath and the $w_{\tau,1}, w_{\tau,2}$ heatbath simultaneously see Proposition (4.5).

The results in Section 2 do not apply when the main particle path is not a Markovian process however the results in Section 3 take correlation into account as long as the correlation is homogeneous. In fact Theorem 3.1 establishes a relationship between the mean particle speed $c^2 = |w_1|^2 = |w_2|^2$, the compound correlation $\rho$, and the mean inter-particle collision time $\tau$. As a result of (4.14b) this exact relationship must hold for for some $c^2 = |w_{\tau,1}|^2 = |w_{\tau,2}|^2$, $\rho'$ and $\tau'$ as well. The results of Section 2 may still provide a good Markovian approximation if the $w_{\tau,1}, w_{\tau,2}$ heatbath renders the pre- and post-collision velocities of the main particle independent.

From section 3 it is clear that the motion for a main particle in the presence of correlation between pre- and post-collision velocities must satisfy a relativistic invariance hence extrapolating from results in Section 2 and Section 4 a proper distribution for the main particle position is likely to satisfy a type of Klein-Gordon equation. This line of research should pursue the ideas of Serva [18] or Guerra [14] and will be investigated in Part II of this paper.

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APPENDIX A.

Proof of Theorem 2.5. Equations (2.14b) can of course be verified by direct substitution however the following simple argument is more intuitive. Using $p_1 =
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$M v_1, p_2 = M v_2, q_1 = M w_1$ and $q_2 = M w_2$ it follows from equation (2.6) that

$$q_2 + q_1 = p_1 \gamma \sin(\theta) - q_1 (\cos(\theta) - 1)$$

$$= p_1 \gamma \sin(\theta) + q_1 2 \sin(\theta/2)^2$$

$$= 2 p_1 \gamma \sin(\theta/2) \cos(\theta/2) + 2 q_1 \sin(\theta/2)^2,$$

so

$$\frac{q_2 + q_1}{2} = \sin(\theta/2) (p_1 \gamma \cos(\theta/2) + q_1 \sin(\theta/2)).$$

Similarly using momentum conservation $p_2 - p_1 = -(q_2 - q_1)$ and equation (2.6) results in

$$\gamma \frac{q_2 - q_1}{2} = \frac{\gamma}{2} p_1 (1 - \cos(\theta)) - q_1 \frac{1}{2} \sin(\theta)$$

$$= p_1 \gamma (\sin(\theta/2)^2 - q_1 \sin(\theta/2) \cos(\theta/2))$$

$$= \sin(\theta/2) (\gamma p_1 \sin(\theta/2) - q_1 \cos(\theta/2)),$$

and adding the squares results in

$$\left| \frac{q_2 + q_1}{2} \right|^2 + \gamma^2 \left| \frac{q_2 - q_1}{2} \right|^2$$

$$= \gamma^2 \sin(\theta/2)^2 \left( |p_1|^2 + \left| \frac{q_1}{\gamma} \right|^2 \right)$$

$$= 2 M H_k \gamma^2 \sin(\theta/2)^2 = \frac{2 M \gamma^4}{1 + \gamma^2} H_k.$$

Substituting

$$q_2 - q_1 = p_1 - p_2,$$

$$q_2 + q_1 = \gamma^2 (p_1 + p_2),$$

into this yields

$$\gamma^4 \left| \frac{p_2 + p_1}{2} \right|^2 + \gamma^2 \left| \frac{p_2 - p_1}{2} \right|^2 = \frac{2 M \gamma^4}{1 + \gamma^2} H_k,$$

hence

$$\left| \frac{p_2 + p_1}{2} \right|^2 + \frac{1}{\gamma^2} \left| \frac{p_2 - p_1}{2} \right|^2 = \frac{2 M}{1 + \gamma^2} H_k,$$

which covers the first two expressions in Theorem (2.5). Now dividing this equation by $M^2$ yields

$$\left| \frac{v_2 + v_1}{2} \right|^2 + \frac{1}{\gamma^2} \left| \frac{v_2 - v_1}{2} \right|^2 = \frac{2}{M(1 + \gamma^2)} H_k = \frac{2}{M_T} H_k,$$

proving equation (2.7a).

Direct substitution can be employed again to obtain equation (2.7b) but this equation can be derived more organically from the pre- and post-collision total kinetic energy and equation (2.7a).
So for a direct derivation write

\[ H_k = \frac{M}{2} |v_2|^2 + \frac{\gamma^2}{2} |w_2|^2 \]  
(A.1a)

\[ = \frac{M(1 + \gamma^2)}{2} \left( \left| \frac{v_2 + v_1}{2} \right|^2 + \frac{1}{2\gamma^2} \left| \frac{v_2 - v_1}{2} \right|^2 \right) \]  
(A.1b)

\[ = \frac{M}{2} \left( |v_1|^2 + \gamma^2 |w_1|^2 \right), \]  
(A.1c)

so that

\[ M(1 + \gamma^2) \left( \left| \frac{v_2 + v_1}{2} \right|^2 + \frac{1}{2\gamma^2} \left| \frac{v_2 - v_1}{2} \right|^2 \right) \]

\[ = \frac{M}{2} (|v_2|^2 + |v_1|^2) + M\gamma^2 |w_1|^2 + \frac{M\gamma^2}{2} \left( |w_2|^2 - |w_1|^2 \right), \]

which is achieved by adding (A.1a) and (A.1c) and equating that to twice the middle term (A.1b).

Carrying the \( v_2, v_1 \) terms to the left hand side then yields

\[ \frac{M(1 + \gamma^2)}{4} \left( |v_2|^2 + |v_1|^2 \right) \left( 1 + \frac{1}{\gamma^2} \right) + \frac{2\gamma^2}{2} v_2^T v_1 \left( 1 - \frac{1}{\gamma^2} \right) \]

\[ - \frac{M}{2} (|v_2|^2 + |v_1|^2) \]

\[ = M(1 + \gamma^2) \left( |v_2|^2 + |v_1|^2 \right) + 2v_2^T v_1 \left( 1 - \frac{1}{\gamma^2} \right) \]

\[ - \frac{M}{2} (|v_2|^2 + |v_1|^2) \]

\[ = M\gamma^2 |w_1|^2 + \frac{M\gamma^2}{2} \left( |w_2|^2 - |w_1|^2 \right). \]

Dividing both sides of this expression by \( \frac{M(1 + \gamma^2)}{4} \) yields

\[ \left( |v_2|^2 + |v_1|^2 \right) \left( 1 + \frac{1}{\gamma^2} \right) + 2v_2^T v_1 \left( 1 - \frac{1}{\gamma^2} \right) \]

\[ - \frac{2}{1 + \gamma^2} (|v_2|^2 + |v_1|^2) \]

\[ = \frac{4\gamma^2}{1 + \gamma^2} |w_1|^2 + \frac{2\gamma^2}{1 + \gamma^2} \left( |w_2|^2 - |w_1|^2 \right), \]

or

\[ \left( |v_2|^2 + |v_1|^2 \right) \left( 1 + \frac{1}{\gamma^2} - \frac{2}{1 + \gamma^2} + 2v_2^T v_1 \left( 1 - \frac{1}{\gamma^2} \right) \]

\[ = \frac{4\gamma^2}{1 + \gamma^2} |w_1|^2 + \frac{2\gamma^2}{1 + \gamma^2} \left( |w_2|^2 - |w_1|^2 \right). \]

Now the constant in this equation can be written as

\[ \left( 1 + \frac{1}{\gamma^2} - \frac{2}{1 + \gamma^2} \right) = \frac{1 + \gamma^4}{\gamma^2 (1 + \gamma^2)}. \]
so that
\[
\left( |v_2|^2 + |v_1|^2 \right) \left( \frac{1 + \gamma^4}{\gamma^2 (1 + \gamma^2)} \right) + 2v_2^T v_1 \left( 1 - \frac{1}{\gamma^2} \right)
\]
\[
= \frac{4\gamma^2}{1 + \gamma^2} |w_1|^2 + \frac{2\gamma^2}{1 + \gamma^2} \left( |w_2|^2 - |w_1|^2 \right).
\]
Dividing by \(\frac{1 + \gamma^4}{1 + \gamma^2}\) yields
\[
\left( \left( |v_2|^2 + |v_1|^2 \right) - 2v_2^T v_1 \left( \frac{1 - \gamma^4}{1 + \gamma^4} \right) \right)
\]
\[
= \frac{4\gamma^4}{1 + \gamma^4} |w_1|^2 + \frac{2\gamma^4}{1 + \gamma^4} \left( |w_2|^2 - |w_1|^2 \right),
\]
and if \(\theta^2 = \frac{1 - \gamma^4}{1 + \gamma^4}\) then \(1 - \theta^2 = \frac{2\gamma^4}{1 + \gamma^4}\) and so (A.2) reduces to
\[
\left( \left( |v_2|^2 + |v_1|^2 \right) - 2v_2^T v_1 \theta^2 \right)
\]
\[
= (1 - \theta^2) \left( 2 |w_1|^2 + \left( |w_2|^2 - |w_1|^2 \right) \right).
\]
Some further rewriting shows that
\[
\frac{(1 - \theta^2)}{2} |v_2 + v_1|^2 + \frac{(1 + \theta^2)}{2} |v_2 - v_1|^2
\]
\[
= (1 - \theta^2) \left( 2 |w_1|^2 + |w_2|^2 - |w_1|^2 \right),
\]
or
\[
|v_2 + v_1|^2 + \frac{(1 + \theta^2)}{(1 - \theta^2)} |v_2 - v_1|^2
\]
\[
= 2 \left( 2w_1^2 + (w_2^2 - w_1^2) \right),
\]
so that finally
\[
\frac{|v_2 + v_1|^2}{2} + \frac{1}{\gamma^2} \frac{|v_2 - v_1|^2}{2}
\]
\[
= \frac{1}{2} \left( |w_1|^2 + |w_1|^2 \right),
\]
since \(\frac{1 + \theta^2}{1 - \theta^2} = \frac{1}{\gamma^2}\). This concludes the proof.

APPENDIX B.

Proof of Theorem (2.1). This Theorem can be generalized slightly to the case where \(M\) and \(m\) are matrices. So if the collision matrix can be written as \(\Gamma = (P \ O \ V \ G)\) then the solution to equations (2.4) equal

\[
P = X(m, M) + (M + Mm^{-1}M)^{-\frac{1}{2}} UY(m, M)^{\frac{1}{2}},
\]
\[
G = X(M, m) + (m + mM^{-1}m)^{-\frac{1}{2}} UY(M, m)^{\frac{1}{2}},
\]
\[
V = m^{-1}M(I - P),
\]
\[
Q = M^{-1}m(I - S),
\]
(B.1)
with

\[ X(m, M) = (M + m)^{-1}M, \]
\[ Y(m, M) = M - Mm^{-1}M \]
\[ + X(m, M)^T (M + Mm^{-1}M) X(m, M). \]

This reduces to (2.5) if \( M \) and \( m \) become diagonal. Notice that solution (2.5) can also be written as

\[ P = \cos\left(\frac{\theta}{2}\right)^2 (I - \gamma^2U), \]
\[ Q = \sin\left(\frac{\theta}{2}\right)^2 (I + U), \]
\[ V = \cos\left(\frac{\theta}{2}\right)^2 (I + U), \]
\[ G = \sin\left(\frac{\theta}{2}\right)^2 \left(I - \frac{1}{\gamma^2}U\right), \]
\[ U^T U = I. \]

To prove that (2.5) and (B.1) above are solutions to equations (2.4a - 2.4c) notice that (2.4a) is equivalent to

\[ V = m^{-1}M(I - P). \]

Substituting that into \( P^T MP + V^T mV = M \) yields

\[ P^T MP + (I - P)^T Mm^{-1}M(I - P) = M, \]

or

\[ P^T (M + Mm^{-1}M)P - P^T Mm^{-1}M \]
\[ - Mm^{-1}MP + Mm^{-1}M = M, \]

so that finally

\[ (P - X)^T (M + Mm^{-1}M)(P - X) = Y, \tag{B.2} \]

with

\[ X(m, M) = (M + Mm^{-1}M)^{-1}Mm^{-1}M = (m + M)^{-1}M, \]
\[ Y(m, M) = M - Mm^{-1}M \]
\[ + X(m, M)^T (M + Mm^{-1}M)^{-1}X(m, M). \]

The solution to equation (B.2) equals

\[ P = X(m, M) + (M + Mm^{-1}M)^{-\frac{1}{2}}UY(m, M)^{\frac{1}{2}}, \tag{B.3} \]

and \( V \) follows from \( V = m^{-1}M(I - P) \) so that

\[ V = m^{-1}M \left(I - X(m, M) - (M + Mm^{-1}M)^{-\frac{1}{2}}UY(m, M)^{\frac{1}{2}}\right) \]
\[ = m^{-1}M \left((m + M)^{-1}m - (M + Mm^{-1}M)^{-\frac{1}{2}}UY(m, M)^{\frac{1}{2}}\right), \tag{B.4} \]

Specifically if \( M = MI, m = mI \) (i.e. the matrices \( m, M \) equal the constant masses \( m, M \) times the unit matrix \( I \)) then (B.2) simplifies to

\[ P^T P - \frac{\sin(\theta)}{2\gamma} (P^T + P) + \cos(\theta)I = 0. \]

Then

\[ \left(P - \frac{\sin(\theta)}{2\gamma}\right)^T \left(P - \frac{\sin(\theta)}{2\gamma}\right) - \frac{\gamma^2 \sin^2(\theta)}{4} I = 0, \]
since
\[
\frac{\sin^2(\theta)}{4\gamma^2} - \gamma^2 \frac{\sin^2(\theta)}{4} = \left(\frac{1}{1 + \gamma^2}\right)^2 - \frac{\gamma^4}{(1 + \gamma^2)^2} = \cos(\theta)
\]
Equation (B.3) then simplifies to
\[
P = \frac{\sin(\theta)}{2\gamma} (I - \gamma^2 U),
\]
for some unitary matrix \(U\) and so equation (B.4) for the matrix \(V\) reduces to
\[
V = \frac{\sin(\theta)}{2\gamma} (I + U).
\]

Using the same approach the matrix \(G\) can be calculated as
\[
G = X(M, m) + (m + mM^{-1}m)^{-\frac{1}{2}} U^\top Y(M, m)^{\frac{1}{2}},
\]
for another arbitrary unitary matrix \(U\). Again, if \(M = MI, m = mI\) (i.e. the matrices \(m, M\) equal the constant masses \(m, M\) times the unit matrix \(I\)), then
\[
G = \frac{\gamma \sin(\theta)}{2} \left( I - \frac{1}{\gamma^2} V \right),
\]
\[
Q = \frac{\gamma \sin(\theta)}{2} (I + V).
\]
Finally from the fourth equation
\[
0 = \frac{\sin^2(\theta)}{4} (1 + \gamma^2) (I - U^\top U),
\]
from which follows \(UU^\top = I\) so that \(U = U^\top\) (\(U\) and \(U^\top\) are unitary) and the proof is complete.

Proof of Theorem (4.1). Using (2.2) and denoting \(\Delta^+ v = v_2 + v_1, \Delta^- v = v_2 - v_1\) it is clear that
\[
\begin{pmatrix}
\Delta^+ v \\
\Delta^- v
\end{pmatrix} =
\begin{pmatrix}
v_2 + v_1 \\
v_2 - v_1
\end{pmatrix} =
\begin{pmatrix}
P + I & Q \\
P - I & Q
\end{pmatrix}
\begin{pmatrix}
v_1 \\
w_1
\end{pmatrix},
\]
so inverting yields
\[
\begin{pmatrix}
v_1 \\
w_1
\end{pmatrix} =
\begin{pmatrix}
P + I & Q \\
-Q & Q
\end{pmatrix}^{-1}
\begin{pmatrix}
\Delta^+ v \\
\Delta^- v
\end{pmatrix},
\]
which can be entered into the total kinetic energy expression \(\mathcal{H}_k = v_1^2 + w_1^2 = v_2^2 + w_2^2\) once the inverse of this matrix has been determined. Since \(P + Q = I\) it is clear that \(P + Q + I = 2I\) so some manipulation shows that
\[
\begin{pmatrix}
P + I & Q \\
-Q & Q
\end{pmatrix}^{-1} = \frac{1}{2}
\begin{pmatrix}
I & -I \\
2Q^{-1} & -I
\end{pmatrix}.
\]
Hence
\[
\begin{pmatrix}
P^T + I & -Q^T \\
Q^T & Q^T
\end{pmatrix}^{-1}
\begin{pmatrix}
I & 0 \\
0 & \gamma^2
\end{pmatrix}
\begin{pmatrix}
P + I & Q \\
-Q & Q
\end{pmatrix}^{-1}
\]
\[
= \begin{pmatrix}
I & I \\
-I & (2Q^{-T} - I)
\end{pmatrix}
\begin{pmatrix}
I & 0 \\
0 & \gamma^2
\end{pmatrix}
\begin{pmatrix}
I & -I \\
-I & (2Q^{-1} - I)
\end{pmatrix}
\]
\[
= \begin{pmatrix}
(1 + \gamma^2)I & -I + \gamma^2V_T \\
-I + \gamma^2V_T & I + \gamma^2V_T^T V_T
\end{pmatrix}
\]
where \( V_T = (2Q^{-1} - I) \).

As a result
\[
\frac{8\mathcal{H}_k}{M} = (v_1^T \quad w_1^T)
\begin{pmatrix}
I & 0 \\
0 & \gamma^2
\end{pmatrix}
\begin{pmatrix}
v_1 \\
w_1
\end{pmatrix}
\]
\[
= (\Delta^+ v^T \quad \Delta^- v^T)
\begin{pmatrix}
I & \gamma^2 I \\
-I & \gamma^2 V_T
\end{pmatrix}
\begin{pmatrix}
I & -I \\
-I & (2Q^{-1} - I)
\end{pmatrix}
\]
\[
= (\Delta^+ v^T \quad \Delta^- v^T)
\begin{pmatrix}
(1 + \gamma^2)I & -I + \gamma^2V_T \\
-I + \gamma^2V_T & I + \gamma^2V_T^T V_T
\end{pmatrix}
\begin{pmatrix}
\Delta^+ v \\
\Delta^- v
\end{pmatrix}
\]
\[
= (1 + \gamma^2)\Delta^+ v^T \Delta^- v - 2\Delta^+ v^T (I - \gamma^2V_T) \Delta^- v
\]
\[
+ \Delta^- v^T (I + \gamma^2V_T^T V_T) \Delta^- v
\]
\]
(B.10)

To further simplify the appearance of this expression the following Lemma is required.

**Lemma B.1.** Let \( Z \) be the collision scattering matrix \( Z = I - 2(I + U)^{-1} = I - \gamma \sin(\theta)Q^{-1} \) with \( U \) the unitary matrix and \( Q \) defined in equation (B.7). Then it is true that
\[
Q^{-1} = \frac{1 + \gamma^2}{\gamma^2} (I + U)^{-1},
\]
(B.11a)
\[
Q^{-T} + Q^{-1} = \frac{2}{\gamma \sin(\theta)} I,
\]
(B.11b)

and
\[
Z^{-T} + Z^{-1} = 0,
\]
(B.12a)
\[
1 - \gamma^2V_T = Z
\]
(B.12b)
\[
\frac{1 + \gamma^2V_T^T V_T}{1 + \gamma^2} = \frac{1}{\gamma^2} I + \frac{1 + \gamma^2}{\gamma^2} Z^T Z.
\]
(B.12c)

**Proof.** Using result (2.5) it is clear that
\[
U = \frac{2}{\gamma \sin(\theta)} Q - I = \frac{1 + \gamma^2}{\gamma^2} Q - I
\]
for the unitary matrix \( U \). Hence,
\[
I = U^T U = \left( \frac{2}{\gamma \sin(\theta)} Q - I \right)^T \left( \frac{2}{\gamma \sin(\theta)} Q - I \right)
\]
\[
= \frac{4Q^T Q}{\gamma^2 \sin^2(\theta)} - \frac{2}{\gamma \sin(\theta)} (Q^T + Q) + I,
\]
so that
\[ \frac{2Q^TQ}{\gamma \sin(\theta)} = (Q^T + Q). \]
Multiplying left with matrix $Q^{-T}$ and right with matrix $Q^{-1}$ it follows that
\[ \frac{2}{\gamma \sin(\theta)} I = (Q^{-T} + Q^{-1}), \]
which demonstrates equation (B.11).
Substituting definition $Q^{-1} = (I - Z)/(\gamma \sin(\theta))$ into (B.11) yields
\[ \frac{2}{\gamma \sin(\theta)} I = \left( \frac{(I - Z)^T}{\gamma \sin(\theta)} + \frac{(I - Z)}{\gamma \sin(\theta)} \right), \]
which demonstrates equation (B.11). From which follows
\[ Z^T + Z = 0 \text{ proving (B.12a) and equation (B.12b) follows from} \]
\[ (I - \gamma^2 V_{\Gamma}) = I - \gamma^2 \left( \frac{2(1 + \gamma^2)}{\gamma^2} (I + U)^{-1} - I \right) \]
\[ = (I + \gamma^2) (I - 2(I + U)^{-1}) \]
\[ = (I + \gamma^2) (I - \gamma \sin(\theta)Q^{-1}) = (1 + \gamma^2) Z. \]
Finally to demonstrate (B.12c) use the definition $V_{\Gamma} = 2Q^{-1} - I$ again to show that
\[ V_{\Gamma} = 2 \left( \frac{I - Z}{\gamma \sin(\theta)} \right) - I = \frac{2}{\gamma \sin(\theta)} I - I - 2 \frac{Z}{\gamma \sin(\theta)} \]
\[ = \frac{1}{\gamma^2} (I - (1 + \gamma^2) Z), \]
so that
\[ I + \gamma^2 V_{\Gamma}^T V_{\Gamma} = 1 + \frac{1}{\gamma^2} (I - (1 + \gamma^2) Z^T) (I - (1 + \gamma^2) Z) \]
\[ = \frac{(1 + \gamma^2)}{\gamma^2} I + \frac{(1 + \gamma^2)^2}{\gamma^2} (Z^T Z) \]
\[ = \frac{(1 + \gamma^2)}{\gamma^2} (I + (1 + \gamma^2) (Z^T Z)), \]
which concludes the Lemma.

Applying (B.12a), (B.12b) to (B.10) yields
\[ \frac{8H_k}{M_T} = \Delta^+ v^T \Delta^+ v - 2 \Delta^+ v^T \left( \frac{I - \gamma^2 V_{\Gamma}}{1 + \gamma^2} \right) \Delta^- v \]
\[ + \Delta^- v^T \left( \frac{I + \gamma^2 V_{\Gamma}^T V_{\Gamma}}{1 + \gamma^2} \right) \Delta^- v \]
\[ = \Delta^+ v^T \Delta^+ v - 2 \Delta^+ v^T Z \Delta^- v + \frac{1}{\gamma^2} \Delta^- v^T \Delta^- v \]
\[ + \left( \frac{1 + \gamma^2}{\gamma^2} \right) \Delta^- v^T Z^T Z \Delta^- v, \]
which is equivalent to equation (4.1) and this concludes the proof.
The total kinetic energy $H_k$ can also be expressed in terms of the velocities of the heatbath particle and the same random matrix $Z$ as is shown in the following Theorem.

**Theorem B.2.** The combined energy of the main and colliding heatbath particle $H_k$ can be expressed as

$$\frac{8H_k}{M_F} = \Delta^+ w^T \Delta^+ w - 2\Delta^+ w^T Z \Delta^- w + \gamma^2 \Delta^- w^T \Delta^- w + (1 + \gamma^2) \Delta^- w^T Z^T Z \Delta^- w,$$

where

$$\Delta^+ w = w_2 + w_1,$$
$$\Delta^- w = w_2 - w_1.$$

As previously the anti-symmetric matrix $Z$ is defined as $Z = I - 2(I + U)^{-1} = I - \gamma \sin(\theta) Q^{-1}$ with $U$ a unitary matrix and $Q$ as defined in (2.5).

**Proof.** Using (4.1) again it is clear that

$$\begin{pmatrix} \Delta^+ w \\ \Delta^- w \end{pmatrix} = \begin{pmatrix} w_2 + w_1 \\ w_2 - w_1 \end{pmatrix} = \begin{pmatrix} V & G + I \\ V & G - I \end{pmatrix} \begin{pmatrix} v_1 \\ w_1 \end{pmatrix} = \begin{pmatrix} V & G + I \\ V & -V \end{pmatrix} \begin{pmatrix} v_1 \\ w_1 \end{pmatrix},$$

so that

$$\begin{pmatrix} v_1 \\ w_1 \end{pmatrix} = \begin{pmatrix} V & G + I \\ V & -V \end{pmatrix}^{-1} \begin{pmatrix} \Delta^+ v \\ \Delta^- v \end{pmatrix}.$$  

As before use $V + G = I$ so that $V + G + I = 2I$ to show that the inverse can be calculated as follows

$$\begin{pmatrix} V & G + I \\ V & -V \end{pmatrix}^{-1} = \frac{1}{2} \begin{pmatrix} I & (2V^{-1} - I) \\ I & -I \end{pmatrix} = \frac{1}{2} \begin{pmatrix} I & X \\ I & -I \end{pmatrix},$$

with $X = (2V^{-1} - I)$ so that

$$\begin{pmatrix} V^T & V^T \\ G^T + I & -V^T \end{pmatrix}^{-1} \begin{pmatrix} I & 0 \\ 0 & \gamma^2 \end{pmatrix} \begin{pmatrix} V & G + I \\ V & -V \end{pmatrix}^{-1}$$

$$= \begin{pmatrix} I & I \\ X^T & -I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \gamma^2 \end{pmatrix} \begin{pmatrix} I & X \\ I & -I \end{pmatrix}$$

$$= \begin{pmatrix} (1 + \gamma^2) I & X - \gamma^2 I \\ X^T - \gamma^2 I & X^T X + \gamma^2 I \end{pmatrix}.$$  

(B.14)
Hence
\[
\frac{8\mathcal{H}_k}{M} = (v_1^T \ w_1^T) \begin{pmatrix} I & 0 \\ 0 & \gamma^2 I \end{pmatrix} \begin{pmatrix} v_1^T \\ w_1^T \end{pmatrix} \\
= \begin{pmatrix} \Delta^+ w^T & \Delta^- w^T \end{pmatrix} \begin{pmatrix} (1 + \gamma^2) I & X - \gamma^2 I \\ X^T - \gamma^2 I & X^T X + \gamma^2 I \end{pmatrix} \begin{pmatrix} \Delta^+ w \\ \Delta^- w \end{pmatrix}
\]
(B.15)

To further simplify the appearance of this expression the following Lemma is required.

**Lemma B.3.** Using the same definition as in Lemma [B.1](#) let \( V^{-1} = \gamma^2 Q^{-1} = \frac{2\sin(\theta)}{(I + U)^{-1}} = \gamma(I - Z)/(\sin(\theta)) \) with \( U \) the unitary matrix and using equation (B.11) it follows that
\[
V^{-1} = (1 + \gamma^2) (I + U)^{-1},
\]
(B.16a)
\[
V^{-T} + V^{-1} = \frac{2\gamma}{\sin(\theta)} I,
\]
(B.16b)

and
\[
\frac{\gamma^2 I - X}{1 + \gamma^2} = Z,
\]
(B.16c)
\[
\frac{X^T X + \gamma^2 I}{1 + \gamma^2} = (1 + \gamma^2) Z^T Z + \gamma^2 I.
\]
(B.16d)

**Proof.** Using \( V^{-1} = \gamma^2 Q^{-1} \), equations (B.16a) and (B.16b) follow immediately from (B.11a) and (B.11b). Now \( X = 2V^{-1} - I = 2\gamma^2 Q^{-1} - I \), hence
\[
(X - \gamma^2 I) = 2 (1 + \gamma^2) (I + U)^{-1} - (1 + \gamma^2) I \\
= (1 + \gamma^2) (2(I + U)^{-1} - I) \\
= - (1 + \gamma^2) Z,
\]
so that \( X = \gamma^2 I - (1 + \gamma^2) Z \) which proves (B.16c). Then finally
\[
X^T X + \gamma^2 I \\
= (\gamma^2 I - (1 + \gamma^2) Z)^T (\gamma^2 I - (1 + \gamma^2) Z) + \gamma^2 I \\
= (1 + \gamma^2)^2 Z^T Z + \gamma^2 (1 + \gamma^2) I,
\]
since \( Z^T + Z = 0 \). This concludes the proof to the Lemma. \( \square \)

Applying expressions (B.16a), (B.16d) to (B.15) yields
\[
\frac{8\mathcal{H}_k}{M} = \Delta^+ w^T \Delta^+ w - 2\Delta^+ w^T Z \Delta^- w \\
+ \gamma^2 \Delta^- w^T \Delta^- w + (1 + \gamma^2) \Delta^- w^T Z^T Z \Delta^- w,
\]
which is equivalent to equation (B.13) and this concludes the proof of the Theorem. \( \square \)
Appendix C.

Proof of Theorem 4.3. This argument is a variation on the proofs presented by E. Nelson [7] and E. Carlen [12]. To prove Theorem 2.12 express the probability of the particle position as \( \rho = \rho(x, t) \), \( x \in \mathbb{R}^n \) for an appropriate (smoothly) differentiable function \( R = R(x, t) \), \( x \in \mathbb{R}^n \) such that \( \rho = e^{2\gamma R/\sigma^2} = e^{2\delta R/\eta} \). Then introduce the sufficiently smooth functions \( A = A(x, t), S = S(x, t), x \in \mathbb{R}^n \) and constants \( \delta, \xi \) to express the backward and forward drifts \( b^+ = b^+(x, t), b^- = b^-(x, t), x \in \mathbb{R}^n, t > 0 \) as follows

\[
\begin{align*}
2\gamma \delta \nabla R &= \sigma^2 \frac{\nabla \rho}{\rho} = b^+ - b^-, \quad (C.1a) \\
2 \xi \left( \nabla S - A \right) &= b^+ + b^-, \quad (C.1b)
\end{align*}
\]

or equivalently

\[
\begin{align*}
b^+ &= \xi \left( \nabla S - A \right) + \gamma \delta \nabla R, \\
b^- &= \xi \left( \nabla S - A \right) - \gamma \delta \nabla R. \quad (C.2)
\end{align*}
\]

Equation (C.1a) is a consequence of equation (1.18c) and the fact that \( \rho = e^{2\gamma R/\sigma^2} \) while equation (C.1b) supplies a definition for the functions \( A = A(x, t), S = S(x, t), x \in \mathbb{R}^n \).

Using this definition equation (4.4) becomes equivalent to

\[
\begin{align*}
E \left[ H_k + \Phi_p \right] \\
\quad = \frac{1}{M_T} E \left[ \xi^2 \left| \nabla S - A \right|^2 - 2 \xi \delta \gamma \left( \nabla S - A \right)^T \nabla R \\
\quad + \delta^2 \nabla R^T \Gamma \nabla R \right] + \frac{n \sigma^2}{2 \gamma} E \left[ \text{Tr} \left( \Gamma^2 \right) \right] + \frac{1}{M_T} E \left[ \Phi_p \right]. \quad (C.3)
\end{align*}
\]

where \( \Gamma^2 = I + (1 + \gamma^2) E \left[ ZZ^T \right] \) and where \( Z \) is the collision scattering matrix such that \( E[Z] = \mathbb{Z} \). The time derivative of this functional depends on the continuity equation (1.19c) which demands that

\[
\rho_t = -\nabla \cdot \left( \frac{b^+ + b^-}{2} \rho \right) = -\xi \nabla \cdot \left( \left( \nabla S - A \right) \rho \right),
\]

where \( \eta = \sigma^2/\gamma \) and \( \rho = e^{2\gamma R/\sigma^2} = e^{2\delta R/\eta} \).

From this follows

\[
\begin{align*}
R_t &= -\frac{\eta \xi}{2\delta} \left( S_{x_ix_j} - A_{x_j} \right) - \xi \left( S_{x_j} - A_j \right) R_{x_j}, \\
R_{tx_k} &= \left( -\frac{\eta \xi}{2\delta} \left( S_{x_ix_j} - A_{x_j} \right) - \xi \left( S_{x_j} - A_j \right) R_{x_j} \right)_{x_k} \quad (C.4)
\end{align*}
\]

using Einstein’s convention for the summation of indices. This abbreviates \( S_{x_ix_j} := \Delta_x S \left( \frac{\partial^2 S}{\partial x_1^2} + \ldots + \frac{\partial^2 S}{\partial x_n^2} \right) \) and \( A_{x_j} := \sum_j A_{x_j} = A_{x_1} + \ldots A_{x_n} \).
Taking the time derivative of the kinetic part of the Hamiltonian \( \mathcal{H}_T \) using (C.4) and ignoring the trace term results in

\[
\frac{d}{dt} \left( \frac{1}{2} \mathcal{H}_T \right) = \frac{1}{2} \int \rho_t \left( \xi^2 (S_{x_j} - A_j) (S_{x_j} - A_j) - 2\xi^2 \delta \gamma (S_{x_j} - A_j) Z_{jk} R_{x_k} \right) \, dx
\]

so with rearranging this reduces to

\[
\frac{d}{dt} \left( \frac{1}{2} \mathcal{H}_T \right) = \frac{1}{2} \int \rho \left( \xi^2 (S_{x_j} - A_j) (S_{x_j} - A_j) - 2\xi^2 \delta \gamma (S_{x_j} - A_j) Z_{jk} R_{x_k} \right) \, dx
\]

(a)

\[
- \xi \delta \gamma \int \rho \left( (S_{x_j,t} - \dot{A}_j) \bar{Z}_{jk} R_{x_k} + (S_{x_j} - A_j) \bar{Z}_{jk} R_{x_k} \right) \, dx
\]

(b)

\[
+ \int \rho \left( \delta^2 R_{x_j} \Gamma_{jk}^x R_{x_k} + \frac{1}{2} \delta^2 R_{x_j} \Gamma_{jk}^x R_{x_k} \right) \, dx.
\]

(c)

The first term becomes

\[
\text{(a)} = \frac{1}{2} \int \frac{2\delta}{\eta} \rho R_t \left( \xi^2 (S_{x_j} - A_j) (S_{x_j} - A_j) - 2\xi^2 \delta \gamma (S_{x_j} - A_j) Z_{jk} R_{x_k} \right) \, dx
\]

\[
= \frac{\delta}{\eta} \int \rho \left( \frac{\xi^2 (S_{x_j} - A_j) (S_{x_j} - A_j) - 2\xi^2 \delta \gamma (S_{x_j} - A_j) Z_{jk} R_{x_k}}{\delta^2 R_{x_j} \Gamma_{jk}^x R_{x_k}} \right) \, dx
\]

\[
= -\frac{\xi}{2} \int \rho \left( (S_{x_j,x} - A_{px}) (S_{x_j} - A_j) \right) \left( \xi^2 (S_{x_j} - A_j) (S_{x_j} - A_j) \right) \, dx
\]

\[
- \frac{\xi \delta}{\eta} \int \rho \left( (S_{x_j} - A_j) R_{x_j} \right) \left( (S_{x_j} - A_j) \right) \, dx
\]

so with one partial integral this reduces to

\[
\text{(a)} = \frac{\xi}{2} \int \rho \left( (S_{x_j} - A_j) \right) \left( \xi^2 (S_{x_j} - A_j) (S_{x_j} - A_j) \right) \, dx
\]

\[
+ \frac{\xi}{2} \int \rho \left( (S_{x_j} - A_j) \right) \left( (S_{x_j} - A_j) \right) \, dx
\]
\[-\frac{\xi\delta}{\eta} \int \rho \left( (S_{x_p} - A_p) \rho \left( \frac{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)}{\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}} \right) \right) dx,\]

or

\[(a) = \frac{\xi}{2} \int \rho \left( (S_{x_p} - A_p) \left( \frac{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)}{\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}} \right) \right) dx
+ \frac{\xi}{2} \int \frac{2\delta}{\eta} \rho R_{x_p} \left( (S_{x_p} - A_p) \left( \frac{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)}{\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}} \right) \right) dx
- \frac{\xi\delta}{\eta} \int \rho \left( (S_{x_p} - A_p) \left( \frac{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)}{\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}} \right) \right) dx,
\]

so that finally

\[(a) = \frac{\xi}{2} \int \rho \left( (S_{x_p} - A_p) \left( \frac{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)}{\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}} \right) \right) dx.
\]

Now the third term becomes

\[(c) = \int \rho \left( \frac{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)}{\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}} \right) \left( \frac{-\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}}{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)} \right) \right) dx
+ \frac{\xi}{2} \int \rho \left( \frac{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)}{\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}} \right) \left( \frac{-\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}}{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)} \right) \right) dx.
\]

This can be written as

\[(c) = \int \rho \left( \frac{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)}{\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}} \right) \left( \frac{-\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}}{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)} \right) \right) dx
+ \frac{\xi}{2} \int \rho \left( \frac{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)}{\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}} \right) \left( \frac{-\delta^2 R_{x_j} \Gamma_{jk}^z R_{x_k}}{\xi^2 (S_{x_1} - A_1) (S_{x_1} - A_1)} \right) \right) dx.
\]
and with one partial integral again this becomes

\[
(c) = \int \rho \left( \frac{\xi^2}{2} (S_{x,j} - A_j) \left( S_{x,t} - \dot{A}_j \right) + \frac{1}{2} \delta^2 R_{x,j} \Gamma_{jk} R_{x k} + \frac{2\xi}{\eta} R_{x k} \left( \delta^2 R_{x,j} \Gamma_{jk} - \xi \delta \gamma (S_{x,j} - A_j) Z_{jk} \right) x_{x k} \right) (S_{x,p} - A_p) R_{x p} \left( S_{x,p} - A_p \right) \right) dx
\]

So then combining the \(a\), \(b\) and \(c\) terms results in

\[
(a) + (b) + (c)
\]

\[
= \int \rho \left( \frac{\xi^2}{2} (S_{x,j} - A_j) \left( S_{x,t} - \dot{A}_j \right) + \frac{1}{2} \delta^2 R_{x,j} \Gamma_{jk} R_{x k} + \frac{2\xi}{\eta} R_{x k} \left( \delta^2 R_{x,j} \Gamma_{jk} - \xi \delta \gamma (S_{x,j} - A_j) Z_{jk} \right) x_{x k} \right) (S_{x,p} - A_p) R_{x p} \left( S_{x,p} - A_p \right) \right) dx
\]

which reduces to

\[
(a) + (b) + (c)
\]

\[
= \int \rho \left( \frac{\xi^2}{2} (S_{x,j} - A_j) \left( S_{x,t} - \dot{A}_j \right) + \frac{1}{2} \delta^2 R_{x,j} \Gamma_{jk} R_{x k} \right) dx
\]

\[
- \xi \int \rho \left( S_{x,p} - A_p \right) R_{x k} \left( \delta^2 R_{x,j} \Gamma_{jk} - \xi \delta \gamma (S_{x,j} - A_j) Z_{jk} \right) x_{x k} \left( S_{x,p} - A_p \right) \right) dx
\]

\[
- \frac{\eta \xi}{2\delta} \int \rho \left( S_{x,p} - A_p \right) \left( \delta^2 R_{x,j} \Gamma_{jk} - \xi \delta \gamma (S_{x,j} - A_j) Z_{jk} \right) x_{x k} \left( S_{x,p} - A_p \right) \right) dx
\]

\[
- \xi \delta \gamma \int \rho \left( \left( S_{x,j} - A_j \right) Z_{jk} R_{x k} + \left( S_{x,j} - A_j \right) Z_{jk} R_{x k} \right) \right) dx,
\]
\[ + \frac{\xi}{2} \int_{-\infty}^{\infty} \rho (S_{2p} - A_p) \left( \frac{\xi^2}{2} \left( S_{x_j} - A_j \right) \left( S_{x_j} - A_j \right) \right) \, dx. \]

Gathering terms finally shows that
\[
\frac{d}{dt} \left( \int \left( \xi |\nabla S - A|^2 - 2\xi \delta \gamma (\nabla S - A)^T \nabla R \right) \right) + \delta^2 \nabla R^T \Gamma^z \nabla R = \xi \int \rho \left( S_{x_p} - A_p \right) \left( \frac{\xi S_i}{2} \left( S_{x_j} - A_j \right) \left( S_{x_j} - A_j \right) \right) \, dx
\]
\[ - \xi^2 \int \rho \left( S_{x_p} - A_p \right) \dot{A}_p + \frac{\eta \delta}{2} \int \rho \left( \delta^2 R_{x_i} \Gamma_{jk} \, R_{x_k} \right) \, dx
\]
\[ + \frac{\eta \delta}{2} \int \rho \left( S_{x_p} - A_p \right) \left( \left( \delta^2 \gamma (\nabla S - A) \nabla R \right) \dot{x_p} \right) \, dx
\]
\[ - \xi \delta \gamma \int \rho \left( (S_{x_j} - A_j) \nabla R_{x_k} + \left( S_{x_j} - A_j \right) \nabla R_{x_k} \right) \, dx. \]  

(C.5)

Now the static potential term time derivative \( \frac{1}{M_T} \frac{d}{dt} E [\Phi_p] \) contains the differential \( \frac{\xi}{M_T} E \left( (\nabla S - A)^T \dot{A} \right) \). The assumption on the potential turns it into a full differential and the \( A \) term disappears if \( \xi = \frac{1}{M_T} \). Once the term with the Trace of the \( \Gamma^z \) matrix is reintroduced the Theorem is proved.

Therefore a sufficient condition for the Hamiltonian in proposition (4.10) to become time-independent the integrand in (4.10) is to equal zero. The following proposition shows that this is equivalent to demanding that the probability for the main particle position \( \rho(x, t) \) is derived from a wave function satisfying Schrödinger's equation.

**Proposition C.1.** Assume that \( Z \equiv 0 \) so that \( E [ZZ^T] \equiv 0, E[Z] \equiv 0, \Gamma^z = I \) and let the potential \( \Phi_p \) satisfy (4.10). \( \psi \) the wave function
\[ \psi = \psi(x, t) = e^{i \int R(z, \chi) \frac{\delta (S(z, \chi))}{\delta z}}, \]

with \( \rho(x, t) = |\psi(x, t)|^2 \). Then equation
\[ \xi^2 (S_t - A_t) - \frac{\delta^2}{2} |\nabla R|^2 + \frac{\xi^2}{2} |\nabla S - A|^2 - \frac{\eta \delta}{2} \Delta_x R + \frac{1}{\xi M_T} \phi = 0, \]

(C.6)

makes the energy terms invariant. Here \( \Delta_x = \left( \frac{\delta^2}{\delta x_1}, \ldots, \frac{\delta^2}{\delta x_n} \right) \). Now this equation is equivalent to
\[ i \chi \dot{\psi} = - \frac{1}{2M_T} \left( \chi \nabla - i A \right)^2 \psi + \phi(x, t) \psi, \]

with \( \chi = M_T \eta \) and \( \delta = \xi = 1/M_T \) so that \( \psi = \psi(x, t) = e^{R(z, \chi) \frac{\delta (S(z, \chi))}{\delta z}} \).
Proof. The proof involves a straightforward verification of equation (4.11) by brute force. Taking derivatives

\[ \eta \frac{\eta}{t} \psi = \psi \left( -i \delta R_t + \xi S_t \right), \]
\[ \eta \frac{\eta}{2} \psi_{x_j} = \frac{1}{2} \psi \left( \delta R_{x_j} + i \xi S_{x_j} \right), \]
\[ \eta \frac{\eta}{2} \psi_{x_j x_j} = \frac{1}{2} \psi \left( \delta R_{x_j x_j} + i \xi S_{x_j x_j} \right), \]
\[ i \xi \eta A_{x_j} \psi_{x_j} = \psi \left( -i \delta \xi A_{x_j} R_{x_j} + A_{x_j} \xi^2 S_{x_j} \right), \]

which combined becomes

\[ \eta \frac{\eta}{t} \psi - \eta \frac{\eta}{2} \psi_{x_j x_j} + i \xi \eta A_{x_j} \psi_{x_j} + \frac{1}{2} |A|^2 \xi^2 \psi + \frac{\xi \eta}{2} i A_{x_j} \psi \]
\[ = -i \psi \left( \delta R_t - \xi A_{x_j} R_{x_j} + \delta \xi R_{x_j} S_{x_j} - \eta \frac{\xi}{2} A_{x_j} + \frac{\eta \xi}{2} S_{x_j} \right) \]
\[ + \left( \xi S_t - \frac{\delta^2}{2} |\nabla R|^2 + \frac{\xi^2}{2} |\nabla S - A|^2 - \frac{\eta \delta}{2} R_{x_j x_j} \right) \]
\[ = -\phi \frac{\xi}{M_T} \psi. \]

Now

\[ -\frac{1}{2} \left( \eta \frac{\eta}{2} \psi_{x_j x_j} - i \xi \eta A_{x_j} \psi_{x_j} \right)^2 \psi \]
\[ = -\frac{1}{2} \left( \eta \frac{\eta}{2} \psi_{x_j x_j} - i A_{x_j} \xi \right) \left( \eta \psi_{x_j x_j} - i A_{x_j} \xi \psi \right) \]
\[ = -\frac{1}{2} \left( \eta \frac{\eta}{2} \psi_{x_j x_j} - i A_{x_j} \xi \psi \right) \]
\[ = -\frac{1}{2} \left( \eta \frac{\eta}{2} \psi_{x_j x_j} - i A_{x_j} \xi \psi \right) \]
\[ = -\frac{1}{2} \left( \eta \frac{\eta}{2} \psi_{x_j x_j} + i \xi A_{x_j} \psi_{x_j} + i A_{x_j} \xi \psi_{x_j} + \frac{1}{2} |A|^2 \xi^2 \psi \right) \]
so indeed

\[ i \eta \psi_t = -\frac{1}{2} \left( \eta \nabla - i A \xi \right)^2 \psi + \frac{\phi \xi}{M_T} \psi. \]

Finally, to adjust for the masses, let \( \chi = M_T \eta \) and let \( \xi = 1/M_T \), then

\[ \psi = \psi(x,t) = e^{\frac{R(x,t) + i S(x,t)}{\chi}}, \]

and

\[ i \chi \psi_t = -\frac{1}{2 M_T} \left( \chi \nabla - i A \right)^2 \psi + \phi(x,t) \psi. \]

This proves (C.5). Also quite clearly

\[ b^+(x,t) = \frac{1}{M_T} (\nabla S - A + \gamma R_x), \]
\[ b^-(x,t) = \frac{1}{M_T} (\nabla S - A - \gamma R_x), \]

which proves equation (C.8). □

An immediate conclusion from quantum mechanics is that the mean acceleration of the motion is guided by the potential \( \phi \).
Proposition C.2. Some straightforward derivatives show that
\[
\frac{d^2}{dt^2} E[x(t)] = -\frac{1}{M_T} \int \rho (\nabla \phi) \, dx.
\]

Proof. In addition,
\[
\frac{d}{dt} E[x(t)] = -\xi \int x \nabla \cdot ((\nabla S - A) \rho) \, dx = \xi \int \rho \nabla (S - A) \, dx,
\]
while
\[
\frac{d^2}{dt^2} E[x(t)] = \xi^2 \int \rho \nabla (S - A) \cdot (\Delta_x S - \nabla A) \, dx + \xi \int \rho (\nabla \dot{S} - \dot{A}) \, dx
\]
\[
= \xi^2 \int \rho \nabla \left( \xi S_t + \frac{\xi^2}{2} |(\nabla S - A)|^2 \right) \, dx
\]
\[
= \xi^2 \int \rho \nabla \left( \frac{\delta^2}{2} |R|^2 + \frac{\eta \delta}{2} \Delta_x R - \frac{\phi}{M_T} \right) \, dx
\]
\[
= -\frac{1}{M_T} \int \rho (\nabla \phi) \, dx.
\]

□

Now the example (4.1) can be slightly extended in the form of the following Proposition.

Proposition C.3. Consider the two-dimensional case \( n=2 \) and assume that
\[
Z^\pm = \left( \begin{array}{c} 0 \\ \mp \nu \end{array} \right),
\]
so that \( E[ZZ^T] = \nu^2 I \) and \( \Gamma^z = I + (1 + \gamma^2) E[ZZ^T] = (1 + (1 + \gamma^2) \nu^2) I = \sigma^z \nu I \).

Then define the wave function
\[
\psi = \psi(x,t) = e^{i M_T \nu (\nabla \cdot \cdot \cdot + iA)}
\]
with \( \rho(x,t) = |\psi(x,t)|^2 \). Then equation
\[
\xi^2 (S_t - A_t) - \frac{\delta^2 \sigma^2}{2} |\nabla R|^2 + \frac{\xi^2}{2} |\nabla S - A|^2 - \frac{\eta \delta \sigma^2}{2} \Delta_x R + \frac{1}{\xi M_T} \phi = 0,
\] (C.7)

makes the energy terms invariant. Here \( \Delta_x = \left( \frac{\partial^2}{\partial x_1^2}, \ldots, \frac{\partial^2}{\partial x_n^2} \right) \). Now this equation is equivalent to
\[
i \chi \psi_t = -\frac{1}{2 M_T} (\chi \nabla - i A)^2 \psi + \phi(x,t) \psi
\] (C.8)

with \( \chi = M_T \eta / \sigma_v, \xi = 1/M_T \) and \( \delta = 1 / (\sigma_v M_T) \).

Proof. Let the wave function \( \psi = \psi(x,t,\xi,\chi) \) satisfy equation (C.7). Then it is clear that the wave function \( \psi' = \psi(x,t,\frac{\delta}{\sigma_v},\xi,\frac{\phi}{\sigma_v}) \) satisfies equation (C.7) above. □
Appendix D.

Proof of Proposition (4.5). Move all the main particle terms in equation (2.2) to the left and all heatbath particle terms to the righthand side (reference also equation (2.5)) to obtain
\[
\begin{pmatrix}
I - P \\
0 - R
\end{pmatrix}
\begin{pmatrix}
v_2 \\
v_1
\end{pmatrix}
=
\begin{pmatrix}
0 & Q \\
-I & S
\end{pmatrix}
\begin{pmatrix}
w_2 \\
w_1
\end{pmatrix},
\] (D.1)
and using remark (2.2) this can be reduced to
\[
\begin{pmatrix}
v_2 \\
v_1
\end{pmatrix}
\begin{pmatrix}
v_1 \\
v_2
\end{pmatrix}
=
\begin{pmatrix}
I - P \\
0 - R
\end{pmatrix}^{-1}
\begin{pmatrix}
0 & Q \\
-I & S
\end{pmatrix}
\begin{pmatrix}
w_2 \\
w_1
\end{pmatrix}
\] (D.2)

Using the collision scattering matrix \((I - Z) = 2\gamma^2 \left( \frac{1}{1+\gamma^2} \right) Q^{-1}\) the expression above reduces to
\[
\begin{pmatrix}
v_2 \\
v_1
\end{pmatrix}
\begin{pmatrix}
v_1 \\
v_2
\end{pmatrix}
=
\gamma \sin(\theta)
\begin{pmatrix}
\cos(\theta) & 1 \\
1 & \cos(\theta)
\end{pmatrix}
\begin{pmatrix}
w_2 \\
w_1
\end{pmatrix}
\] + \gamma \sin(\theta)
\begin{pmatrix}
-Z & Z \\
-Z & Z
\end{pmatrix}
\begin{pmatrix}
w_2 \\
w_1
\end{pmatrix},
\] (D.3)

where \(-mW = \frac{1+\gamma^2}{2} mZ(w_2 - w_1) = \frac{1+\gamma^2}{2} mZ \Delta - w\) is the additional momentum transfer from the heatbath to the main particle. Notice the rather interesting fact that this allows (D.3) to be rewritten as follows
\[
\begin{pmatrix}
v_2 \\
v_1
\end{pmatrix}
\begin{pmatrix}
w_2 + W \\
w_1 + W
\end{pmatrix},
\] (D.4)

since the vector \((W)\) is an eigenvector of the matrix \(\gamma \sin(\theta)
\begin{pmatrix}
\cos(\theta) & 1 \\
1 & \cos(\theta)
\end{pmatrix}\). This is in fact equivalent to equation (4.16).

Now returning to (D.2)
\[
\begin{pmatrix}
v_2 \\
v_1
\end{pmatrix}
\begin{pmatrix}
v_1 \\
v_2
\end{pmatrix}
=
\gamma \sin(\theta)
\begin{pmatrix}
\cos(\theta) & 1 \\
1 & \cos(\theta)
\end{pmatrix}
\begin{pmatrix}
w_2 \\
w_1
\end{pmatrix},
\] so that
\[
\begin{pmatrix}
w_2 \\
w_1
\end{pmatrix}
\begin{pmatrix}
w_1 \\
w_2
\end{pmatrix}
=
\frac{\sin(\theta)}{\gamma}
\begin{pmatrix}
\cos(\theta)I - Z & I + Z \\
-I - \cos(\theta)I + Z
\end{pmatrix}
\begin{pmatrix}
v_2 \\
v_1
\end{pmatrix}
\]
\[
=
\frac{1}{\gamma \sin(\theta)}
\begin{pmatrix}
-I - \cos(\theta)I - Z & I + Z \\
-I - \cos(\theta)I + Z
\end{pmatrix}
\begin{pmatrix}
v_2 \\
v_1
\end{pmatrix}.
\]
Then
\[
E \left[ \begin{pmatrix} \Delta^+_{\frac{\tau_2}{\tau_1}} & \Delta^-_{\frac{\tau_2}{\tau_1}} \end{pmatrix} \begin{pmatrix} \Delta^+_{\frac{\tau_2}{\tau_1}} & \Delta^-_{\frac{\tau_2}{\tau_1}} \end{pmatrix} \right]
\]
\[
= \frac{2\sigma^2}{\tau_\gamma \sin^2(\theta)} \begin{pmatrix} (1 + \cos^2(\theta))I & -2\cos(\theta)I \\ -2\cos(\theta)I & (1 + \cos^2(\theta))I \end{pmatrix}
\]
\[
+ \frac{2\sigma^2}{\tau_\gamma \sin^2(\theta)} \begin{pmatrix} E[ZZ^T] & \Omega \\ \Omega^T & E[ZZ^T] \end{pmatrix},
\]
where
\[
\Omega = (1 - \cos(\theta)I) \bar{Z} + E[ZZ^T].
\]
Recombining the \(\cos(\theta)^2\) and \(\sin(\theta)^2\) terms in the first matrix (refer to Theorem (2.8)) this reduces to
\[
E \left[ \begin{pmatrix} \Delta^+_{\frac{\tau_2}{\tau_1}} & \Delta^-_{\frac{\tau_2}{\tau_1}} \end{pmatrix} \begin{pmatrix} \Delta^+_{\frac{\tau_2}{\tau_1}} & \Delta^-_{\frac{\tau_2}{\tau_1}} \end{pmatrix} \right]
\]
\[
= \frac{\sigma^2}{\tau\alpha^2} \left( \begin{pmatrix} 1 & -\left(1 - 2\alpha^2\right) \\ -\left(1 - 2\alpha^2\right) & 1 \end{pmatrix} \right) + \Gamma_Z,
\]
with
\[
\Gamma_Z = \frac{2\sigma^2}{\tau_\gamma \sin^2(\theta)} \begin{pmatrix} E[ZZ^T] & \Omega \\ \Omega^T & E[ZZ^T] \end{pmatrix}.
\]
Clearly here \(\Gamma_Z\) is positive definite and symmetric. This concludes the proof.