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The Motion of a Tracer Particle in a One-Dimensional System: Analysis and Simulation

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Abstract

Our goal is to obtain a test system for the evaluation of time-stepping methods in molecular dynamics. We consider a family of deterministic systems consisting of a finite number of particles interacting on a compact interval. The particles are given random initial conditions and interact through instantaneous energy- and momentum-conserving collisions. As the number of particles, the particle density, and the mean particle speed go to infinity, the trajectory of a tracer particle is shown to converge to a stationary Gaussian process. We simulate the system with two numerical methods, one symplectic, the other energy-conserving, and assess the methods' ability to recapture the system's limiting statistics.

1 Introduction

In the field of molecular dynamics, researchers use numerical integrators to approximate the motion of systems of particles. They integrate over long periods of time and extract statistical information from the computed trajectories. This, in turn, can be used to determine macroscopic properties of the system. For optimal efficiency, they integrate using as long a step-length as possible while still maintaining the stability of the computed solution. In this regime trajectories are not computed accurately. Nevertheless, it is observed that statistical features of solutions are maintained in some circumstances. (See [1],[3].)

One possible explanation for this phenomenon is the existence of an underlying stochastic process [11]. Suppose that the trajectories of the deterministic process approximate some stochastic process in the sense of distribution. If we use a numerical method whose trajectories also approximate the same stochastic process, then the numerical solution will have similar statistical features to the original system, even though there is no path-wise agreement.

The goal of this paper is to construct a test case for this situation. We seek a deterministic system having a component of its trajectory that approximates a well-understood stochastic process. Once given such a system, we can use it to test numerical integrators. We integrate the system with the integrator using step-lengths that do not resolve the trajectories correctly. Then we can investigate how accurately these computed solutions reproduce the statistical features of the underlying stochastic process.

Our construction is inspired by a 1968 paper of Spitzer [12] that provides an example of a sequence of deterministic systems whose trajectories converge to a stochastic process. He shows that Brownian motion can be obtained as the limit of a sequence of deterministic processes on the real line with random initial conditions. His construction consists of placing point particles on the real line according to a Poisson distribution. Then each particle is assigned a random velocity independently of the other particles. The particles are allowed to move, so that they interact through energy- and momentum-conserving collisions: i.e., whenever two particles meet, there is an instantaneous collision in which they exchange velocities. A single particle is placed at the origin and its subsequent trajectory observed. Spitzer proves that with an appropriate scaling of the variables, the path of this tracer particle converges weakly to standard Brownian motion.

There are two difficulties with using this system for our investigations. The first is that since it is infinite in extent, it is impossible to simulate it completely on a computer. As a way of avoiding this difficulty, in Section 2 we introduce a finite counterpart to Spitzer's result. We describe a sequence of systems each consisting of a finite number of particles interacting on a compact segment of the real line. In Section 3 we prove that as the number of particles goes to infinity, the trajectory of a tracer particle will converge to a stationary Gaussian process with a known correlation function.

The second difficulty is that neither Spitzer's system nor the system we present in Section 2 are described purely in terms of ordinary differential equations, since the inter-particle collisions are instantaneous. Thus we cannot use these systems as test problems for numerical integrators without dealing with the issues of collision detection. However, we show in Section 4 how we can approximate the non-differentiable flow of these systems with the flow of a differential equation by replacing the hard, instantaneous collisions of the particles with collisions mediated by a soft potential. This system approximates the non-differentiable system in the limit as the stiffness of the inter-particle forces goes to infinity. If we allow both the number of particles and the inter-particle stiffness to go to infinity with a particular scaling, we conjecture the the tracers trajectory converges to the same Gaussian process. We show the results of some numerical experiment which support this statement.

We conclude is Section 5 by showing the results of some numerical experiments conducted with the systems described in Section 4. We apply two numerical methods to the system: the symplectic Euler method and the symplectic Euler method projected after each step to conserve energy. We simulate the system of ODEs with these methods for increasing number of particles and inter-particle stiffness. We observe that the former method, which is symplectic, computes the limiting statistical properties of the trajectory of the tracer particle quite well for large time step. The projected method does not have as good performance for steplengths of comparable size.

Other researchers have continued with Spitzer's ideas in [12] in other directions. One possibility is to allow the mass of the tracer to differ from the mass of the other particles. In [7] Holley proves that with such a scaling the trajectory of the tracer particle weakly converges to the Ornstein-Uhlenbeck process. In [8] Mürmann takes this result further by proving a similar result when the collisions between the particles do not occur instantly but are mediated by a soft potential.

2 Particle Systems on a Compact Interval

In this section we describe a sequence of particle systems on the interval $[-1,1]$. For each odd positive integer n, the system will consist of n interacting particles. We let the tracer particle be the "median" particle in the interval, that is, the one with an equal number of particles above and below it. When we scale the system by a factor of $n^{1/2}$ we will see that the trajectory of this tracer particle will converge to a Gaussian random process.

Let q_i, $i = 1, \ldots, n$ be i.i.d. random variables, each uniformly distributed on $[-1,1]$. These are the initial positions of the n particles. We give the particles i.i.d. velocities p_i according to a distribution with a probability density f. We make the following assumptions on f.

Assumptions 2.1 *The probability density f satisfies*
(i) f is symmetric: $f(-p) = f(p)$.
(ii) f is L_1 and nontrivial: $\mathbb{E}|p_i| > 0$.
(iii) For some $C > 0$, $\int_K^\infty f(p)dp \leq CK^{-2}$ for all $K > 0$.

Given these initial conditions, we allow the particles to move according to the following rules. Particles move at constant velocity until they encounter either another particle or one of the barriers at -1 or 1. If two particles collide, the particles merely exchange velocities. If a particle hits a wall, it reverses its velocity. These rules are a natural consequence of assuming that the total energy of the system is conserved and that when two particles collide, their total momentum is conserved. With these rules for motion we designate the position at time t of the particle starting at q_i by $x_i(t)$. Note that the order of the particles is unchanged in time. By this we mean that if $q_i < q_j$ then $x_i(t) \leq x_j(t)$ for all $t \geq 0$. Choose m so that q_m is the median of the $\{q_i\}$. It follows that $x_m(t)$ is the median of the $\{x_i(t)\}$ for all t. We choose this particle to be our tracer particle.

If we multiply the positions of all of the particles over time by $n^{1/2}$, we obtain a system of n particles interacting over the interval $[-n^{1/2}, n^{1/2}]$, with an average particle speed of $n^{1/2}\mathbb{E}|p_i|$. We will denote the position of the tracer particle with this scaling by U_n, so that $U_n(t) = n^{1/2}x_m(t)$ for $t \geq 0$.

In order to get a more convenient representation of the motion of the tracer particle, we now describe a different, but related, set of rules of motion. The rules of motion are the same as before except that the particles do not interact with each other, but only the walls. Thus when the trajectories of two particles intersect, the particles merely pass through each other. Under this set of rules, we designate the position of the particle starting at q_i by $y_i(t)$, for $t \geq 0$. There is a simple expression for $y_i(t)$. If there were no walls, the particle's position at time t would be $q_i + tp_i$. The effect of the walls is to "fold" the particle's trajectory back into the interval $[-1, 1]$. This is accomplished by a function G such that

$$y_i(t) = G(q_i + tp_i). \tag{2.1}$$

G is the periodic function with period 4 such that

$$G(x) = \begin{cases} x, & -1 \leq x \leq 1 \\ 2 - x, & 1 \leq x \leq 3. \end{cases} \tag{2.2}$$

There is a relationship between the two sets of trajectories, $\{x_i(t)\}$ and $\{y_i(t)\}$. At any point in time the set of positions the particles take is the same under the two different rules of motion. Since the position of the tracer particle at any time is given by the median of all the $x_i(t)$, its position is also given by the median of all the $y_i(t)$. So the trajectory of the tracer particle is given by

$$U_n(t) := n^{1/2}x_m(t) = n^{1/2} \operatorname*{med}_{i=1\ldots n}(y_i(t)) = n^{1/2} \operatorname*{med}_{i=1\ldots n}(G(q_i + tp_i)). \tag{2.3}$$

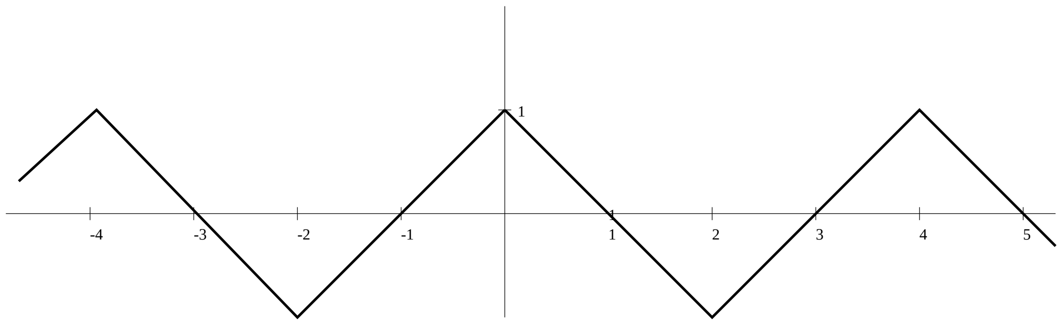

Figure 2.1: The function H.

This is a convenient representation, since $\{q_i\}_{i=1}^n$ and $\{p_i\}_{i=1}^n$ are independent random variables with known distributions.

We now present our main result. It states that as the number of particles, n, goes to infinity the scaled trajectory of the tracer particle will converge to a Gaussian process. This result is the basis for the numerical experiments performed later in the paper. For the statement of the main theorem, we define H to be a periodic function with period 4 such that

$$H(z) = \begin{cases} 1 - z, & 0 \le z \le 2, \\ z - 3, & 2 \le z \le 4 \end{cases} \tag{2.4}$$

as shown in Figure 2.1.

Theorem 2.2 *Let $\{q_i\}_{i\ge1}$, $\{p_i\}_{i\ge1}$, be mutually independent i.i.d. sequences of random variables, where each q_i is distributed uniformly on $[-1,1]$ and each p_i is distributed with density f satisfying Assumptions 2.1. Then as $n \to \infty$,*

$$U_n(t) := n^{1/2} \operatorname*{med}_{i=1\ldots n} (G(q_i + tp_i)) \Rightarrow U(t)$$

where $U(t)$ is the stationary continuous mean-zero Gaussian process with covariance

$$C(t) := \mathbb{E}[U(0)U(t)] = \int_{-\infty}^{\infty} H(pt)f(p)dp. \tag{2.5}$$

The convergence is in the weak sense on $\mathrm{C}[0,T]$ for any $T > 0$.

We note that we will have completely determined the limiting process since a mean-zero continuous Gaussian process is completely specified by its covariance function. Since our process is stationary we have

$$C(s,t) := \mathbb{E}x(s)x(t) = \mathbb{E}x(0)x(t-s) = C(t-s).$$

Method of Proof. Let us first recall the usual technique for proving weak convergence in $\mathrm{C}[0, T]$, which Spitzer uses for his problem. As explained in Billingsley [2, Ch. 2], one shows that the finite dimensional distributions of U_n weakly converge to the finite dimensional distributions of U and that the set of probability measures for U_n is tight. In proving the tightness condition Spitzer extensively uses the Poisson distribution of the particle positions, which is invariant through all time in his case. Since the distribution of particle positions does not have this Poisson distribution in our case, we cannot follow the same strategy that he did. Indeed, directly proving tightness for the processes $U_n, n \geq 1$ proves to be very difficult. Hence, we approach the problem in a different way.

Rather than prove convergence of U_n to U directly in $\mathrm{C}[0, T]$, we will use the fact that this convergence is equivalent to

$$\mathbb{P}\{U_n \leq X\} \to \mathbb{P}\{U \leq X\} \tag{2.6}$$

for all infinitely differentiable functions X on $[0, T]$. Then we show that this convergence does hold for all such X. This is done by constructing, for each such X, a sequence N_n of what we call *dual processes* in $D[0, T]$. ($D[0, T]$ is the space of all functions that, at each point, are continuous on the right and have a limit on the left.) We show that (2.6) is equivalent to showing that the corresponding N_n weakly converge to U in $D[0, T]$. This, in turn, can be done using the methods of [2, Ch. 3]. It requires that we prove convergence of the finite-dimensional distributions of N_n (Appendix A), and a tightness condition (Appendix B). The structure of these dual processes makes it far easier to prove tightness for them than for the original U_n. To the best of our knowledge, this method is novel for proving weak convergence in $C[0, T]$.

Properties of the Covariance. Since U is a stationary Gaussian process, it is completely specified by its covariance. Equation 2.5 gives the covariance as it depends on the velocity density function f. In Figure 2.2 we show plots of C vs t for two choices of f. The first shows the case when velocities are chosen uniformly in $[-1, 1]$; the second shows the case when they are chosen according to the standard Gaussian distribution.

When we choose velocities to be either -1 or 1, each with probability $1/2$, then $C = H$ defined by (2.4). In this latter case there is no decay of correlation. This occurs because all the particles are moving at speed 1. Since the box has length 2, all particles return to where they were initially after every 4 time units. Thus the auto-covariance must be 1 for every time that is a multiple of 4.

Some calculation shows that the right-derivatives of C at 0 satisfy (for densi-

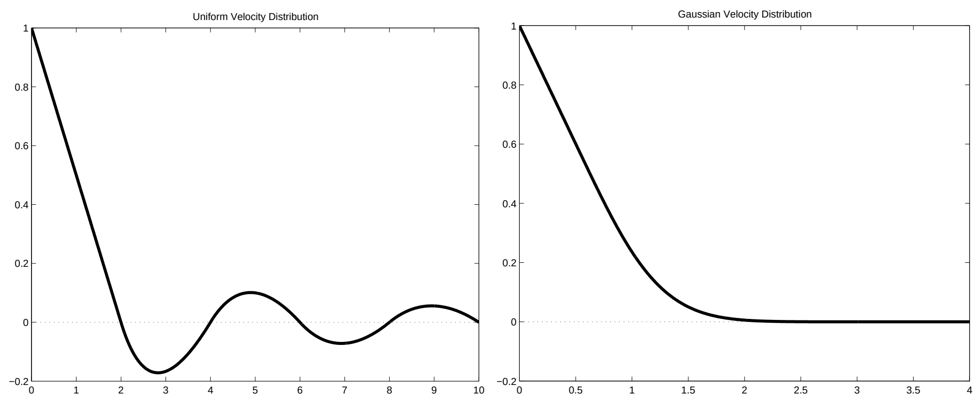

Figure 2.2: Covariance functions for two choices of the velocity distribution.

ties f with bounded second moment [13])

$$C'(0) = -\int_{-\infty}^{\infty} |p| f(p) dp = -\mathbb{E}|p|, \qquad C''(0) = 0. \tag{2.7}$$

From this one can show that for any physically reasonable f, U cannot be a Markov process. This can also be used to prove that there does exist a Gaussian random process U with covariance C.

3 Proof of Main Theorem

To establish the convergence of U_n to U, we need to show that an appropriately scaled median of n i.i.d. random processes converges to a Gaussian process. Thus we can view the main result as a Central Limit Theorem, except that it is for medians, rather than means, and for processes, rather than random variables. There is an extensive literature on asymptotic limits for medians and other central order statistics. The book [10] provides a thorough treatment of the subject. Here, we will extend some techniques in the field to prove the result for our particular random processes. First we need a sufficient condition for weak convergence of functions in $\mathrm{C}[0, T]$.

We use $U \leq X$ for functions in $\mathrm{C}[0, T]$ to denote $U(t) \leq X(t)$ for all $t \in [0, T]$. Define $A_C(X) := \{Y \in \mathrm{C}[0, T] : Y \leq X\}$. We say that X is a continuity point of U if $\mathbb{P}\{U \in \partial A_C(X)\} = 0$. A standard result [2] tells us that if $U_n \Rightarrow U$ then, for all X that are continuity points of U, $\mathbb{P}\{U_n \leq X\} \Rightarrow \mathbb{P}\{U \leq X\}$.

We use a strengthened form of the converse of this fact to establish weak convergence. Here we denote the set of all infinitely differentiable functions on $[0, T]$ by $\mathrm{C}^\infty[0, T]$.

Theorem 3.1 *If $\mathbb{P}\{U_n \le X\} \to \mathbb{P}\{U \le X\}$ for all $X \in \mathrm{C}^\infty[0, T]$ that are continuity points of U, then $U_n \Rightarrow U$.*

Proof This is Exercise 1.2.6 of Billingsley [2, p. 17]. See [13] for a proof. $\square$

To establish the convergence (3.1) we define what we will call the dual process for each X. For each fixed $X \in \mathrm{C}[0, T]$, we define the dual process of U_n to be

$$N_n(t) := n^{-1/2} \sum_{j=1}^{n} \eta_{n,j}(t) \tag{3.8}$$

where

$$\eta_{n,j}(t) := [1 + n^{-1/2}X(t) - 2\mathbf{1}_{y_j(t) \le n^{-1/2}X(t)}] \tag{3.9}$$

for $t \in [0, T]$. Note that this process is not, in general, continuous, nor is it even in $D[0, T]$. However, we will henceforth denote by $\eta_{n,j}$, N_n the versions of the above processes that are in $D[0, T]$.

Theorem 3.2 *For all $X \in \mathrm{C}[0, T]$, the event $\{U_n \le X\}$ is equivalent to the event $\{N_n \le X\}$.*

Proof Here we are following very closely the ideas in Reiss [10] in the proof of the CLT for medians of vectors.

Consider the event of interest:

$$\{U_n \le X\} = \{n^{1/2}Z_n \le X\} = \{Z_n \le n^{-1/2}X\}.$$

Recalling that $Z_n(t)$ is the median of $y_j(t), j = 1, \ldots, n$, we have for each $t \in [0, T]$

$$\{Z_n(t) \le n^{-1/2}X(t)\} = \left\{ \sum_{j=1}^{n} \mathbf{1}_{y_j(t) \le n^{-1/2}X(t)} \ge n/2 \right\},$$

where $\mathbf{1}_A$ is the indicator function of the event A. So

$$\{U_n(t) \le X(t)\} = \left\{ -\sum_{j=1}^{n} \mathbf{1}_{y_j(t) \le n^{-1/2}X(t)} \le -n/2 \right\}.$$

Let us manipulate the event on the right of the equation. We subtract the expectation of the left-hand-side of the inequality from both sides. Since

$$\mathbb{E}\left(-\mathbf{1}_{y_j(t)\le n^{-1/2}X(t)}\right) = -\left(\frac{1+n^{-1/2}X(t)}{2}\right),$$

we get

$$\begin{aligned}
&\{U_n(t) \le X(t)\} \\
&= \left\{\sum_{j=1}^{n}\left[\frac{1+n^{-1/2}X(t)}{2} - \mathbf{1}_{q_j(t)\le n^{-1/2}X(t)}\right] \le \sum_{j=1}^{n}\frac{n^{-1/2}X(t)}{2}\right\} \\
&= \left\{n^{-1/2}\sum_{j=1}^{n}\left[1+n^{-1/2}X(t) - 2\mathbf{1}_{q_j(t)\le n^{-1/2}X(t)}\right] \le X(t)\right\}.
\end{aligned}$$

Recalling the definition of N_n and $\eta_{n,j}$,

$$\{U_n \le X\} = \left\{n^{-1/2}\sum_{j=1}^{n}\eta_{n,j} \le X\right\} = \{N_n \le X\},$$

as required. □

We will also need the following theorem stated in Billingsley [2].

Theorem 3.3 ([2] Theorem 15.6.) *Suppose that the finite dimensional distributions of N_n converge to those of an almost surely continuous process U on $[0,T]$, and that*

$$\mathbb{E}\{|N_n(t)-N_n(t_1)|^\gamma |N_n(t_2)-N_n(t)|^\gamma\} \le (t_2-t_1)^{2\alpha} \tag{3.10}$$

for $t_1 \le t \le t_2$ and $n \ge 1$, where $\gamma \ge 0$, $\alpha > 1/2$. Then $N_n \Rightarrow U$. □

We now establish the limiting behavior of the dual process.

Theorem 3.4 *For each $X \in \mathrm{C}^\infty[0,T]$, $N_n \Rightarrow U$ in $D[0,T]$.*

Proof The convergence of finite-dimensional distributions is proved in Theorem A.1 of Appendix A. The inequality (3.10) is proved in Theorem B.1 of Appendix B. □

Now we can prove our main theorem.

Proof of Theorem 2.2 From Theorem 3.4 we know that $N_n \Rightarrow U$ in $D[0,T]$ for all $X \in \mathrm{C}^\infty[0,T]$. Let $A_D(X) = \{Y \in D[0,T] : Y \leq X\}$. From the properties of weak convergence we know that that for all $X \in \mathrm{C}^\infty[0,T]$ such that $\mathbb{P}\{U \in \partial A_D(X)\} = 0$, we have $\mathbb{P}\{N_n \leq X\} \to \mathbb{P}\{U \leq X\}$.

Let $A_C(X) = \{Y \in \mathrm{C}[0,T] : Y \leq X\}$. We have that

$$\partial A_C(X) = \{Y \in \mathrm{C}[0,T] : Y \leq X, Y(t) = X(t) \text{ for some } t\}.$$

Likewise

$$\partial A_D(X) = \{Y \in D[0,T] : Y \leq X, Y(t) = X(t) \text{ for some } t\}.$$

So $\partial A_C(X) = \partial A_D(X) \cap \mathrm{C}[0,T]$. Since $U \in \mathrm{C}[0,T]$,

$$\mathbb{P}\{U \in \partial A_C(X)\} = \mathbb{P}\{U \in \partial A_D(X)\}.$$

The above considerations show us that if $\mathbb{P}\{U \in \partial A_C(X)\} = 0$ and $X \in \mathrm{C}^\infty[0,T]$ then $\mathbb{P}\{U \in \partial A_D(X)\} = 0$ and hence $\mathbb{P}\{N_n \leq X\} \to \mathbb{P}\{U \leq X\}$. So by Theorem 3.2 we have that

$$\mathbb{P}\{U_n \leq X\} = \mathbb{P}\{N_n \leq X\} \to \mathbb{P}\{U \leq X\}.$$

whenever $X \in \mathrm{C}^\infty[0,T]$ and $\mathbb{P}\{U \in \partial A_C(X)\}$, as required by Theorem 3.1. □

4 Approximation with Soft Collisions

We have now shown that a particular sequence of deterministic processes with random initial conditions has a component $\{U_n\}$, defined by (2.3), that converges to a stochastic process U specified by (2.5). As mentioned earlier, since these deterministic processes are not described purely by ODEs we cannot test ODE solvers on them. So we shall now describe an approximation of these systems by systems of ODEs. We will then provide numerical evidence that the trajectories of the tracer particles of these ODE systems also converges to the stochastic process U in a particular limit.

As before, for each odd positive integer n, we place n particles on the interval $[-n^{1/2}, n^{1/2}]$. Each particle is given a velocity $n^{1/2}p$ where p is selected from the distribution with density f, as before. From now on, we fix f to be the density of the standard Gaussian distribution. We denote the position and velocity of particle i at time t by $q_i(t)$ and $p_i(t)$ respectively. In contrast to the previous case, we describe the motion of the particles through a set of ODEs. The differential equations describing the positions q_i and the momenta p_i are

$$\dot{q}_i(t) = p_i(t), \quad i = 1, \ldots, n,$$

and

$$\begin{aligned}
\dot{p}_1(t) &= -k^2(q_1(t) - q_2(t))_+ + k^2(-n^{1/2} - q_1(t))_+, \\
\dot{p}_i(t) &= -k^2(q_i(t) - q_{i+1}(t))_+ + k^2(q_{i-1}(t) - q_i(t))_+, \quad i = 2, \ldots, n-1, \\
\dot{p}_n(t) &= -k^2(q_n(t) - n^{1/2})_+ + k^2(q_{n-1}(t) - q_n(t))_+,
\end{aligned}$$

where $(x)_+ = \max(0, x)$ for $x \in \mathbb{R}$. This system can be viewed as a Hamiltonian system with Hamiltonian

$$H(q,p) = U(q) + \frac{1}{2}\sum_{i=1}^{n} p_i^2,$$

where

$$U(q) = \frac{1}{2}k^2(-n^{1/2} - q_1)_+^2 + \frac{1}{2}\sum_{i=2}^{n-1} k^2(q_{i-1} - q_i)_+^2 + \frac{1}{2}k^2(q_n - n^{1/2})_+^2.$$

The flow of this system of ODEs is very similar to that of the original process. However, when two particles meet each other, rather than instantaneously exchanging velocities, they are allowed to overlap. While overlapping, they apply a repelling force to each other that is proportional to the amount that they have overlapped. Thus while the particles are in contact, they go through linear harmonic motion. After half a period of this motion, they cease to overlap and have velocities pointing away from each other. Since momentum and energy are conserved, the net effect is that their velocities are exchanged, as in the hard collision case. However, their positions are displaced relative to where they would be after a hard collision.

In the ODEs above k is a constant denoting the stiffness of the repulsion between the particles, and between the particles and the walls. For $k = 0$ the particles do not interact at all; as $k \to \infty$ we expect the trajectories of the system to converge to those of the original system with the same initial data. (See, for example, [9].)

In order to have a sequence of systems of ODEs that converge to the same stochastic process, we allow k to go to infinity as n does. Here, we make the

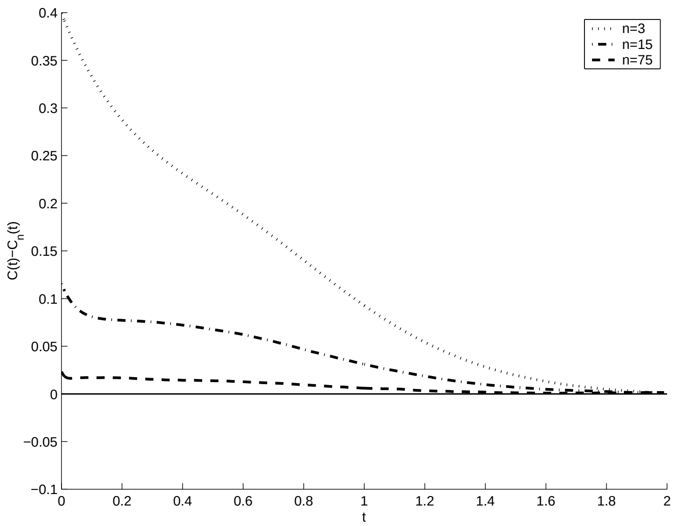

Figure 4.1: $C(t) - C_n(t)$ for $t \in [0, 2]$.

choice $k = n^2$. In this case the duration of a collision between two particles is on the order of n^{-2}. The average length of time between collisions for a single particle is on the order of n^{-1}. So, as we increase n, the collision durations become shorter and shorter with respect to the length of time between collisions, and in the limit of $n \to \infty$ we expect the system to be a close approximation to the system with instantaneous collisions. We conjecture that the ODE system with this choice of k has the same limiting properties as we proved for the instantaneous collision system: the trajectory of the tracer particles weakly converges to U. We now provide some numerical evidence to support this conjecture.

To describe our results, we introduce some notation. As before, C is the covariance of the limiting process U. Define C_n to be the covariance of our original hard particle process with n particles described in Section 2. Our main theorem in Section 3 shows that $C_n(t)$ converges to $C(t)$ for all t. In Figure 4.1 we show the convergence of C_n to C by plotting the difference of the two functions for different values of n. We denote by $C_{n,k}$ the covariance function for the process described by the ODEs with n particles and a stiffness parameter k. A consequence of the softened system converging weakly to U as $n \to \infty$ with $k = n^2$ would be the convergence of $C_{n,k}$ to C. Figure 4.2 shows that this is the case when $k = n^2$. (The figure was obtained by integrating the ODEs with time step Δt, letting $\Delta t = \gamma/k$, and then decreasing γ until there was convergence.) Of

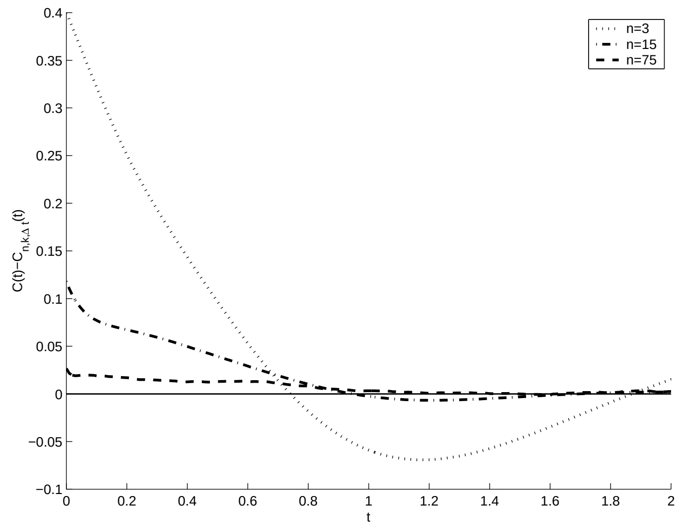

Figure 4.2: $C(t) - C_{n,k}(t)$ for $t \in [0, 4]$ with $k = n^2$. The standard deviation of the error on the curves never exceeds 0.004.

course, convergence of the covariance function does not guarantee convergence of the process, but the evidence partly confirms our hypothesis.

5 Numerical Approximation

In the previous section we presented a sequence of particle systems described by ODEs and parameterized by n, the number of particles, and k the stiffness of the collisions. If we let $k = n^2$, it appears that the trajectory of the tracer particle weakly converges to that of the stochastic process U as n goes to infinity. We will use this scaling numerically integrate the system for increasing values of n, and see how well limiting statistics are reproduced.

The first method we will apply to our system is the symplectic Euler method. Consider the system of ODEs

$$\dot{q} = p, \quad \dot{p} = f(q),$$

where $q, p \in \mathbb{R}^n$. The symplectic Euler method with step length Δt generates a sequence of approximations

$$q_{n+1} = q_n + \Delta t p_n, \quad p_{n+1} = p_n + \Delta t f(q_{n+1}).$$

For this method to stably compute approximations to the system of ODEs, it is necessary that $\Delta t \sim k^{-1}$. Thus a natural place to begin our numerical experiments is to examine how well the symplectic Euler method reproduces the statistics of the large n limit with $\Delta t = \gamma k^{-1}$, for different values of γ. We will denote by $C_{n,k,\Delta t}$ the covariance function computed by the integrator with time step Δt applied to the system of ODEs with parameters n, k.

Figure 5.1 shows $C - C_{n,k,\Delta t}$ computed by the symplectic Euler method with $\Delta t = k^{-1}$, where $k = n^2$ and $n = 3, 15, 75$. The covariance function appears to converge to the limiting covariance function C with this scaling. This property was also observed with $\Delta t = \gamma k^{-1}$ for $\gamma = 0.5, 0.25$. This provides an example of the phenomenon which we hoped to explore. Since with the $\Delta t \sim k^{-1}$ scaling we are not resolving fine details of the collisions, we are not computing trajectories accurately in this limit. Even with $\gamma = 1$, which is close to the largest step size allowed by stability, the limiting statistical properties of the trajectories are computed accurately.

One property of the symplectic Euler method which may be viewed as a drawback for molecular dynamics simulations is that it does not conserve the energy of the system exactly. One way to remedy this is to use a projection method; see [6, IV.4]. A projection method is a modified version of a standard time-stepping algorithm wherein the solution is forced to have the correct energy after each step. This is done by first taking a step with a standard method— which will lead to a value with possibly incorrect energy— and then projecting this value onto the manifold of states with the correct energy.

Typically, projection methods for Hamiltonian systems are implemented as follows. Suppose we are numerically integrating a Hamiltonian system of ODEs on the space of points $x = (q, p) \in \mathbb{R}^{2n}$ with fixed energy $H(x) = H_0$. From a state $x_n = (q_n, p_n)$ with the correct energy a standard time-stepper is used to obtain the state x^*_{n+1}. The gradient of the Hamiltonian is computed at this state: $s = \nabla H(x^*_{n+1})$. Then an $\alpha \in \mathbb{R}$ is computed so that $H(x^*_{n+1} + \alpha s) = H_0$. Then we set $x_{n+1} = x^*_{n+1} + \alpha s$.

In our implementation there are two aspects of this scheme that we modify. Firstly, the we use a different projection direction s. The usual choice,

$$s = \nabla H(q, p) = [\nabla U(q) \quad p]^T ,$$

does not scale well with increasing k. Instead we use

$$s = \left[\nabla U(q) \quad k^2 p\right]^T .$$

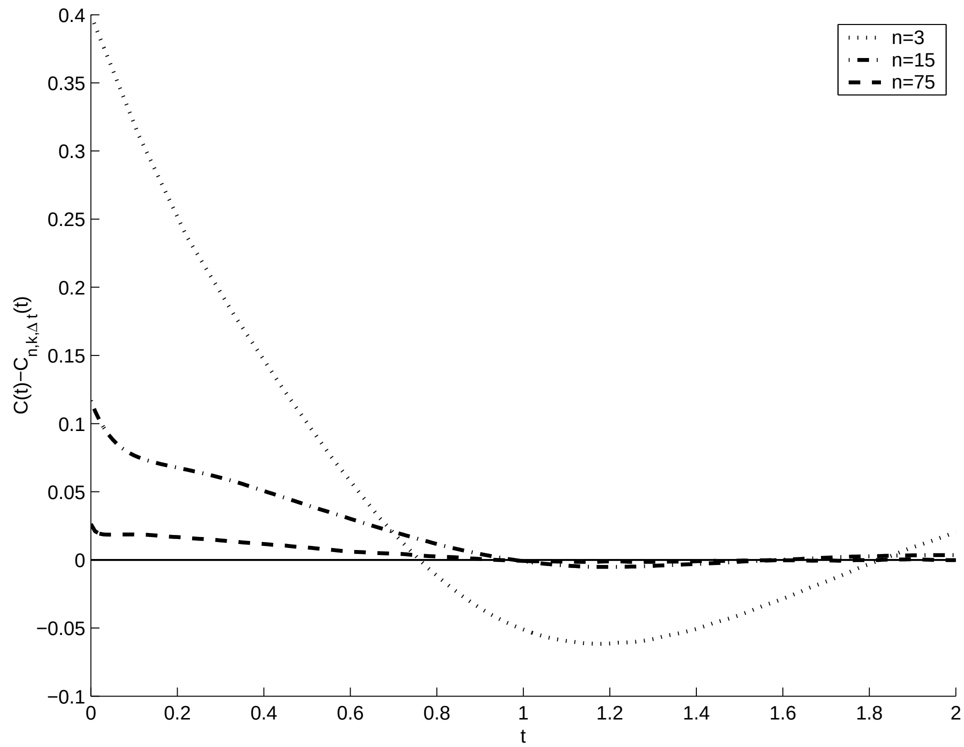

Figure 5.1: Symplectic Euler method. $C(t) - C_{n,k,\Delta t}(t)$ for $t \in [0,2]$, with $\Delta t = k^{-1}$, and $k = n^2$. The standard deviation of the error on the curves never exceeds 0.002.

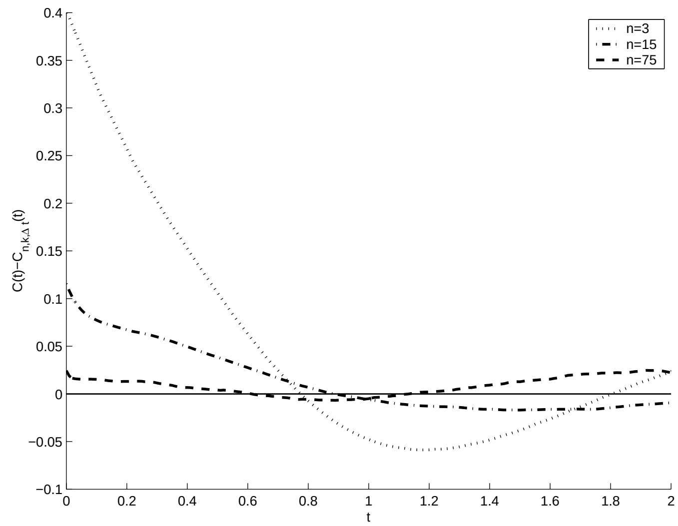

Figure 5.2: Projected symplectic Euler method. $C(t) - C_{n,k,\Delta t}(t)$ for $t \in [0, 2]$ with $k = n^2$ and $\Delta t = k^{-1}$. The standard deviation of the error on the curves never exceeds 0.005.

See [13] for further explanation. Secondly, for our system it is not always possible to find an α that solves the above nonlinear equation. In these rare cases we find an α that locally minimizes the residual of the equation, and then proceed with the projection to $H(x) = H_0$ as usual on subsequent steps.

We take the symplectic Euler method and implement the projection scheme described above in order to make it energy conserving. We will refer to this method as the projected symplectic Euler method. We conduct the same numerical experiments for it as we did for the symplectic Euler method. Figure 5.2 shows $C - C_{n,k,\Delta t}$ computed by this method. As before $\Delta t = k^{-1}$, $k = n^2$, and $n = 3, 15, 75$. Comparison with Figure 5.1 shows that for $n = 3, 15$, the method computes similar covariance functions to those of the non-projected method. However, for $n = 75$ the covariance function appears to diverge from the limit C.

We repeat the experiment with the projected method with a slightly larger timestep: $\Delta t = 1.25k^{-1}$. The results shown are significantly worse than for the previous steplength. The computed covariance function is clear diverging from C as $n \to \infty$.

These studies are preliminary, but they do suggest two lessons: (1) symplecticity is more important than energy conservation for the computation of statistical

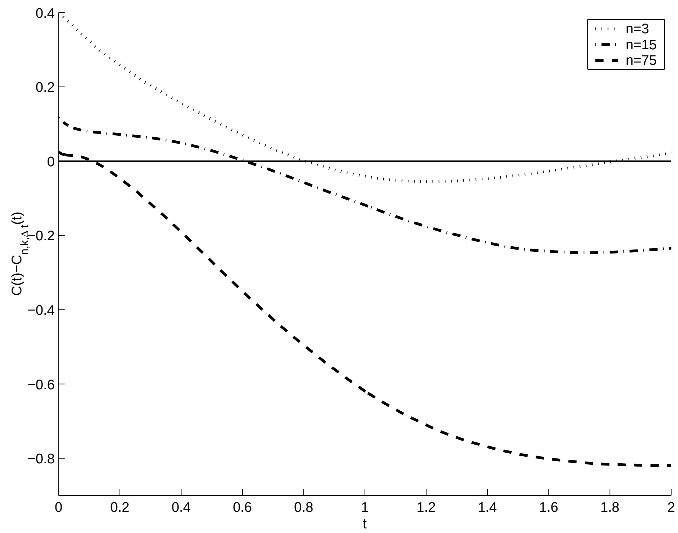

Figure 5.3: Projected symplectic Euler method. $C(t) - C_{n,k,\Delta t}(t)$ for $t \in [0, 2]$ with $k = n^2$ and $\Delta t = 1.25k^{-1}$. The standard deviation of the error on the curves never exceeds 0.005.

properties in molecular dynamics, and (2) projection does not safely allow one to take longer time steps without grossly affecting the quality of the simulation.

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A Finite-Dimensional Distributions of the Dual Process

Theorem A.1 *Recall the definition of N_n from (3.8). For any $t_1, t_2, \dots, t_d \in [0, T]$ the random vector*

$$[N_n(t_1), N_n(t_2), \dots, N_n(t_d)]$$

converges in distribution to a Gaussian random vector with covariance matrix $\Sigma_{ij} = C(t_i - t_j)$. Here, $C(t)$ is as defined in (2.5).

Proof Recall the definition of the process y_j from (2.1). For our later convenience we define

$$F_t(x_1, x_2) := \mathbb{P}\{y_j(0) \leq x_1, y_j(t) \leq x_2\}.$$

It is straightforward to show the for each j, the process y_j is stationary [13]. This implies

$$\mathbb{P}\{y_j(t_1) \leq x_1, y_j(t_2) \leq x_2\} = F_{t_2 - t_1}(x_1, x_2) \tag{A.11}$$

for any $t_1, t_2 \in [0, T]$.

We apply a Central Limit Theorem of Dvoretzky ([4], Theorem 1). The result holds for certain dependent random vector arrays, but we will only need it for the independent case.

Theorem A.2 *(From [4]). For each n, let $X_{n,m}$, $1 \leq m \leq n$ be independent random column vectors with $\mathbb{E}X_{n,m} = 0$. Let Σ be a $k \times k$ matrix. For a vector X, denote its norm by $|X|$ and its transpose by X^T. For an event A, let*

$$\mathbb{E}(X; A) := \mathbb{E}(X\mathbf{1}_A).$$

Suppose

- *(i)* $\lim_{n\to\infty} \sum_{m=1}^{n} \mathbb{E}X_{n,m}X_{n,m}^T = \Sigma$,
- *(ii) for all* $\epsilon > 0$, $\lim_{n\to\infty} \sum_{m=1}^{n} \mathbb{E}(|X_{n,m}|^2; |X_{n,m}| > \epsilon) = 0$.

Then $S_n = X_{n,1} + \cdots + X_{n,n} \Rightarrow \mathcal{N}(0, \Sigma)$ as $n \to \infty$. $\square$

In our case, S_n and $X_{n,j}$ are vectors of length d with $S_{n,k} = N_n(t_k)$ and $X_{n,j,k} = n^{-1/2}\eta_{n,j}(t_k)$, where $\eta_{n,j}$ is defined in (3.9). Recall the definition of $\eta_{n,j}(t)$ in (3.9). We proceed to check the hypotheses of the CLT.

We first need to verify that $\mathbb{E}n^{-1/2}\eta_{n,j}(t_k) = 0$, for each k. We have

$$\mathbb{E}n^{-1/2}\eta_{n,j}(t_k) = n^{-1/2}\left[1 + n^{-1/2}X(t_k) - 2\mathbb{P}\{y_j(t_k) \le n^{-1/2}X(t_k)\}\right] = 0.$$

Furthermore, with some algebra and the fact that

$$\mathbb{E}[\mathbf{1}_{y_j(t)\le n^{-1/2}X(t)}] = (1 + n^{-1/2}X(t_k))/2,$$

we obtain

$$\begin{aligned}
&\sum_{j=1}^{n}\mathbb{E}\left[(n^{-1/2}\eta_{n,j}(t_k))(n^{-1/2}\eta_{n,j}(t_l))\right] \\
&= n^{-1}\sum_{j=1}^{n}[-(1 + n^{-1/2}X(t_k))(1 + n^{-1/2}X(t_l)) \\
&\quad +4\mathbb{P}\{y_j(t_k) \le n^{-1/2}X(t_k), y_j(t_l) \le n^{-1/2}X(t_l)\}] \\
&= 4F_{t_l-t_k}(n^{-1/2}X(t_k), n^{-1/2}X(t_l)) - (1 + n^{-1/2}X(t_k))(1 + n^{-1/2}X(t_l))
\end{aligned}$$

Lemma A.3 shows that F_t is continuous at $(0,0)$ for all $t \in [0,T]$. Hence the above quantity converges to $4F_{t_l-t_k}(0,0) - 1$ as $n \to \infty$. Lemma A.4 shows that $4F_t(0,0) - 1 = C(t)$ for $t \ge 0$ so this is the appropriate covariance as stated in the theorem.

In order to verify the final condition of the CLT theorem, observe that $|\eta_{n,j}(t_k)| \le 2$ for all n, j, k, so

$$\begin{aligned}
&\sum_{j=1}^{n}\mathbb{E}\left[|(n^{-1/2}\eta_{n,j}(t_k))(n^{-1/2}\eta_{n,j}(t_l))|; \sum_{i=1}^{d}|n^{-1/2}\eta_{n,j}(t_i)| > \epsilon\right] \\
&= \sum_{j=1}^{n}n^{-1}\mathbb{E}\left[|\eta_{n,j}(t_k)||\eta_{n,j}(t_l)|; \sum_{i=1}^{d}|\eta_{n,j}(t_i)| > n^{1/2}\epsilon\right] \\
&\le \mathbb{E}\left[4; 2d > n^{1/2}\epsilon\right] = 4\mathbb{P}\{2d > n^{1/2}\epsilon\}
\end{aligned}$$

which converges to zero as required. $\square$

Lemma A.3 *The function* $F_t : \mathbb{R}^2 \to \mathbb{R}$ *is continuous at* $(0,0)$.

Proof This can be proved by showing that F_t is Lipschitz in each each variable at $(0, 0)$. See [13]. $\square$

Lemma A.4 *We have*

$$4F_t(0,0) - 1 = C(t).$$

Proof We can rewrite F_t as

$$\begin{aligned} F_t(z_1, z_2) &= \mathbb{E}[\mathbf{1}_{q \le z_1} \mathbf{1}_{G(q+tp) \le z_2}] \\ &= \tfrac{1}{2} \int_{-\infty}^{\infty} \int_{-1}^{1} \mathbf{1}_{q \le z_1} \mathbf{1}_{G(q+pt) \le z_2} dq f(p)\, dp. \end{aligned} \tag{A.12}$$

So

$$\begin{aligned} 4F_t(0,0) - 1 &= 2 \int_{-\infty}^{\infty} \int_{-1}^{1} \mathbf{1}_{q \le 0} \mathbf{1}_{G(q+pt) \le 0} dq f(p)\, dp - 1 \\ &= 4 \int_{-\infty}^{\infty} \tilde{H}(pt) f(p)\, dp - 1 \end{aligned}$$

where we have defined

$$\tilde{H}(z) := \frac{1}{2} \int_{-1}^{1} \mathbf{1}_{q \le 0} \mathbf{1}_{G(q+z) \le 0} dq. \tag{A.13}$$

In order to obtain a more explicit expression for $\tilde{H}$, we first observe that it will be periodic with a period of 4. Then some lengthy but straightforward calculations will show that

$$\tilde{H}(z) = \begin{cases} (1-z)/2, & 0 \le z \le 1, \\ 0, & 1 \le z \le 2, \\ (z-2)/2, & 2 \le z \le 3, \\ 1/2, & 3 \le z \le 4. \end{cases} \tag{A.14}$$

We can take advantage of the fact that f is symmetric about 0:

$$\begin{aligned} 4F_t(0,0) - 1 &= 4 \int_{-\infty}^{\infty} \tilde{H}(pt)(f(p) + f(-p))/2\, dp - 1 \\ &= 2 \int_{-\infty}^{\infty} (\tilde{H}(pt) + \tilde{H}(-pt)) f(p)\, dp - 1 \\ &= \int_{-\infty}^{\infty} [2(\tilde{H}(pt) + \tilde{H}(-pt)) - 1] f(p)\, dp \end{aligned}$$

The expression in the square brackets happens to equal H of equation (2.4). So

$$4F_t(0,0) - 1 = \int_{-\infty}^{\infty} H(pt) f(p)\, dp = C(t)$$

as required. $\square$

B Tightness of the Dual Process

Remark. Here we establish the tightness criterion (3.10) of Theorem 3.3. It is clear that we only need to prove it for n sufficiently large.

We will use some of the ideas of Hahn [5], where a similar argument is given in order to prove a Central Limit Theorem in $D[0,T]$.

Theorem B.1 *For n sufficiently large*

$$\mathbb{E}|N_n(t) - N_n(t_1)|^2 |N_n(t_2) - N_n(t)|^2 \leq C(t_2 - t_1)^2$$

for $t_1 \leq t \leq t_2$, for some constant C.

Proof Recall that $N_n(t) := n^{-1/2} \sum_{j=1}^n \eta_{n,j}(t)$. Using the independence of the $\eta_{n,j}$ for different j and the fact that increments of $\eta_{n,j}$ have zero mean, we obtain

$$\begin{aligned}
&\mathbb{E}\left[|N_n(t) - N_n(t_1)|^2 |N_n(t_2) - N_n(t)|^2\right] \\
&= n^{-2}\mathbb{E}\left[\sum_j (\eta_{n,j}(t) - \eta_{n,j}(t_1))\right]^2 \left[\sum_j (\eta_{n,j}(t_2) - \eta_{n,j}(t))\right]^2 \\
&= n^{-2}\sum_j \mathbb{E}\left[(\eta_{n,j}(t) - \eta_{n,j}(t_1))^2 (\eta_{n,j}(t_2) - \eta_{n,j}(t))^2\right] \\
&\quad + n^{-2}\sum_{j \neq k} \mathbb{E}\left[(\eta_{n,j}(t) - \eta_{n,j}(t_1))^2\right] \cdot \mathbb{E}[(\eta_{n,k}(t_2) - \eta_{n,k}(t))^2] \\
&\quad + n^{-2}\sum_{j \neq k} \mathbb{E}[(\eta_{n,j}(t) - \eta_{n,j}(t_1))(\eta_{n,j}(t_2) - \eta_{n,j}(t))] \\
&\quad \cdot \mathbb{E}[(\eta_{n,k}(t) - \eta_{n,k}(t_1))(\eta_{n,k}(t_2) - \eta_{n,k}(t))].
\end{aligned}$$

Using the fact that the the $\eta_{n,j}$ are identically distributed processes we obtain that the expectation of interest is

$$
\begin{aligned}
& n^{-1}\mathbb{E}[(\eta_{n,1}(t)-\eta_{n,1}(t_1))^2(\eta_{n,1}(t_2)-\eta_{n,1}(t))^2] \\
& + \quad \frac{n+1}{2n}\mathbb{E}[(\eta_{n,1}(t)-\eta_{n,1}(t_1))^2]\cdot\mathbb{E}[(\eta_{n,1}(t_2)-\eta_{n,1}(t))^2] \\
& + \quad \frac{n+1}{2n}(\mathbb{E}[(\eta_{n,1}(t)-\eta_{n,1}(t_1))(\eta_{n,1}(t)-\eta_{n,1}(t_2))])^2.
\end{aligned}
$$

Using the Cauchy-Schwartz inequality we obtain

$$
\begin{aligned}
& \mathbb{E}\left[|N_n(t)-N_n(t_1)|^2|N_n(t_2)-N_n(t)|^2\right] \\
& \quad \leq \quad \mathbb{E}[(\eta_{n,1}(t)-\eta_{n,1}(t_1))^2(\eta_{n,1}(t_2)-\eta_{n,1}(t))^2] \\
& \qquad\quad +2\mathbb{E}[(\eta_{n,1}(t)-\eta_{n,1}(t_1))^2]\mathbb{E}[(\eta_{n,1}(t_2)-\eta_{n,1}(t))^2].
\end{aligned}
$$

The first term is shown to be $\mathcal{O}(t_2-t_1)^2$ in Lemma B.3. The second term is shown to be smaller than $\mathcal{O}(t_2-t)(t-t_1)\leq\mathcal{O}(t_2-t_1)^2$ in Lemma B.2. So the required bound follows. $\square$

Lemma B.2 *For $s,t\in[0,T]$, $s\leq t$,*

$$
\mathbb{E}(\eta_{n,1}(t)-\eta_{n,1}(s))^2 < C(t-s)
$$

for some positive C.

Proof

$$
\begin{aligned}
& \mathbb{E}(\eta_{n,1}(t)-\eta_{n,1}(s))^2 \\
& \quad = \quad \mathbb{E}(n^{-1/2}(X(t)-X(s))-2\mathbf{1}_{y_1(t)\leq n^{-1/2}X(t)}+2\mathbf{1}_{y_1(s)\leq n^{-1/2}X(s)})^2 \\
& \quad \leq \quad 2n^{-1}(X(t)-X(s))^2+8\mathbb{E}(\mathbf{1}_{y_1(t)\leq n^{-1/2}X(t)}-\mathbf{1}_{y_1(s)\leq n^{-1/2}X(s)})^2
\end{aligned}
$$

Since X is a smooth function on a compact interval, we can uniformly bound the first term by some constant times $(t-s)^2$. The second term is the probability that the relative position of y_1 and $n^{-1/2}X$ will switch from time s to time t. We can bound this by considering the magnitude of the derivatives of the two functions.

The rate of change of y_1 is at most $|p|$, where p is the initial velocity of the first particle. Let χ be the maximum of $|X'|$ on $[0,T]$. Then the rate of change of $n^{-1/2}X$ is certainly no greater than χ. So the relative rate of change of the two functions is at most $|p| + \chi$. For the two functions to cross on the interval $[s, t]$ one or more times we must have

$$|y_1(s) - n^{-1/2}X(s)| \leq (|p| + \chi)(t - s).$$

For this to happen, $y_1(s)$ must fall in an interval of length $2(|p| + \chi)(t - s)$. Since for all s, y_j is uniformly distributed on $[-1, 1]$, conditioning on the value of p gives us that the probability of the event of interest is less than

$$\int_{-\infty}^{\infty} f(p)(|p| + \chi)(t - s)\, dp \leq \chi(t - s)(1 + \int_{-\infty}^{\infty} f(p)|p|\, dp) \leq \quad C(t - s)$$

where C is some constant, since f is L_1 by assumption. $\square$

Lemma B.3 *For $0 \leq t_1 < t < t_2 \leq T$ and for large enough n*

$$\mathbb{E}[(\eta_{n,1}(t) - \eta_{n,1}(t_1))^2(\eta_{n,1}(t_2) - \eta_{n,1}(t))^2] \leq C(t_1 - t_2)^2$$

for some positive C.

Proof

$$\begin{aligned} & \mathbb{E}[(\eta_{n,1}(t) - \eta_{n,1}(t_1))^2(\eta_{n,1}(t_2) - \eta_{n,1}(t))^2] \\ \leq \; & 2\mathbb{E}[\{n^{-1}(X(t) - X(t_1))^2 + (2\mathbf{1}_{y_j(t) \leq n^{-1/2}X(t)} - 2\mathbf{1}_{y_j(t_1) \leq n^{-1/2}X(t_1)})^2\} \cdot \\ & \quad \{n^{-1}(X(t_2) - X(t))^2 + (2\mathbf{1}_{y_j(t_2) \leq n^{-1/2}X(t_2)} - 2\mathbf{1}_{y_j(t) \leq n^{-1/2}X(t)})^2\}]. \end{aligned}$$

If we expand the product out and recall that $X(t) - X(s) = \mathcal{O}(t - s)$ and use the result of Lemma B.2, it only remains to show that

$$\begin{aligned} \mathbb{E}\left[(\mathbf{1}_{y_j(t) \leq n^{-1/2}X(t)} - \mathbf{1}_{y_j(t_1) \leq n^{-1/2}X(t_1)})^2(\mathbf{1}_{y_j(t_2) \leq n^{-1/2}X(t_2)} - \mathbf{1}_{y_j(t) \leq n^{-1/2}X(t)})^2\right] \\ \leq C(t_2 - t_1)^2 \end{aligned}$$

for some constant C. This expectation is equal to

$$\begin{aligned} \mathbb{P}\{\mathbf{1}_{y_j(t) \leq n^{-1/2}X(t)} - \mathbf{1}_{y_j(t_1) \leq n^{-1/2}X(t_1)} \neq 0, \\ \mathbf{1}_{y_j(t_2) \leq n^{-1/2}X(t_2)} - \mathbf{1}_{y_j(t) \leq n^{-1/2}X(t)} \neq 0\}. \end{aligned}$$

For any $t \in [t_1, t_2]$ this probability is strictly less than the probability that the relative positions of y_1 and $n^{-1/2}X$ will switch twice or more during the time interval $[t_1, t_2]$. We must bound the probability of this happening.

We condition on two possible ways for this event to occur. The first way is for y_1 to cross $n^{-1/2}X$ some number of times, then bounce off a wall, then cross $n^{-1/2}X$ again, all within the time period $[t_1, t_2]$. This is where we make an assumption on the size of n. We assume that n is large enough that $\max_{[0,T]} n^{1/2}X(t) < 1/2$. Since the walls are at ± 1, the particle trajectory must travel a distance of at least 1 in the time $t_2 - t_1$ to be able to meet the function, meet a wall, and meet the function again. So the probability of this event is less than

$$\mathbb{P}\{|p| \geq (t_2 - t_1)^{-1}\} \leq \int_{(t_2-t_1)^{-1}}^{\infty} |p| f(p) dp \leq C(t_2 - t_1)^2$$

by the assumptions on f. So this probability is bounded as required.

The other possibility is that, while maintaining its direction, the particle crosses the curve $n^{-1/2}X$ twice or more. Because $X \in \mathrm{C}^\infty[0,T]$, the position and slope of y_1 must be within a very narrow range for such a double crossing to occur. Let us define the slope of y_1 at t_1 to be v. By the Mean Value Theorem, we must have $n^{1/2}X(s) = v$ for some $s \in [t_1, t_2]$. How close must the values $n^{-1/2}X(s)$ and $y_1(s)$ be for there to be a crossing at all?

Consider the function $z(t) = n^{-1/2}X(t) - y_1(t)$ on $[t_1, t_2]$. We have that $z'(s) = 0$ and also that $z(u) = 0$ for some $u \in [t_1, t_2]$, a point where the two functions cross. We have that

$$|z(u) - z(s)| \leq \frac{1}{2}|u - s|^2 \max_{[t_1,t_2]} |z''(t)|$$

If we denote the maximum of the second derivative of X by $\mathcal{X}$, this give us

$$|n^{-1/2}X(s) - y_1(s)| = |z(s)| \leq |t_1 - t_2|^2 \mathcal{X}.$$

So $y_1(u)$ must lie within $\mathcal{X}|t_1 - t_2|^2$ of $n^{-1/2}X(u)$. Since $y_1(u)$ is uniformly distributed on $[-1, 1]$, the probability of the happening is $\mathcal{O}((t_1 - t_2)^2)$ as required. □