
A Semi-realistic Model for Brownian Motion in One Dimension

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Abstract

The phenomenon of Brownian motion, the erratic movement of a microscopically-visible sized particle in a fluid, was first studied in detail around 1830 by the biologist Robert Brown (see [Bro28], [Bro29]). At the beginning of the last century Einstein (see [Ein05], [Ein06]) and v. Smoluchowski (see [vS06]) gave a physical explanation of Brownian motion. A good survey can be found in [Nel67]. However, in a common mathematical model the rigorous mathematical proof that the Brownian particle, which is embedded in an ideal gas, shows diffusive behavior could not be provided so far. It has to be shown that the trajectory of the Brownian particle converges in the diffusive scaling in distribution against a Brownian motion (Wiener process). One of the mathematical difficulties is the fact that the process of the motion of the molecule is not Markovian due to recollisions. In this work we show an analogous result in a simplified model.

We consider a one-dimensional system in equilibrium at temperature T and density ρ consisting of a molecule of mass $M > 0$ embedded in an ideal gas of atoms of mass $m > 0$ ($m < M$). The molecule is confined in the interval $\Lambda \subset \mathbb{R}$ (with elastic reflections at the boundary), whereas the atoms are not confined by the interval and can freely pass the boundary without being affected in any way. Since the position of the molecule is bounded, the position in the diffusive scaling converges to zero. Therefore, a process R_t is constructed which is unbounded and measures in an appropriate sense the distance the molecule would have travelled if it moved without a confinement. We show diffusive behavior for R_t in diffusive scaling. To prove this, we show that the velocity process of R_t fulfills the requirements of the functional Central Limit Theorem (fCLT) of [Dav68] improved by results of [McL75] and [DG86]. An important requirement of the fCLT is that the velocity process is α -mixing. If this property is shown for a Markov process which contains the velocity process, the latter inherits this property. In our case, the Markov process essentially describes the positions and velocities of all particles in Λ .

Making use of a result from [DG86], we show that the diffusion constant is positive.

Zusammenfassung

Das Phänomen der Brownschen Bewegung, die erratische Bewegung mikroskopisch sichtbarer Teilchen in einer Flüssigkeit, wurde erstmals um 1830 von dem Biologen Robert Brown näher untersucht (vgl. [Bro28], [Bro29]). Anfang des letzten Jahrhunderts konnte die Brownsche Bewegung durch Einstein ([Ein05], [Ein06]) und v. Smoluchowski ([vS06]) physikalisch erklärt werden. Eine gute Übersicht findet man in [Nel67]. Jedoch konnte in einem gängigen mathematischen Modell der rigorose mathematische Beweis, dass das Brownsche Teilchen, das in ein ideales Gas eingebettet ist, bisher nicht erbracht werden. Zu zeigen ist, dass die Trajektorie des Brownschen Teilchens in der diffusiven Skalierung in Verteilung gegen eine Brownsche Bewegung (Wiener Prozess) konvergiert. Da der Prozess der Bewegung des Moleküls aufgrund von Rekollisionen kein Markovscher Prozess ist und deswegen mathematisch schwer zu handhaben ist, betrachten wir folgendes Modell, das zwar abgeändert ist, aber durch das dennoch ein analoges Resultat gezeigt werden kann. Wir betrachten ein eindimensionales System im Equilibrium, bestehend aus einem Molekül der Masse $M > 0$, eingebettet in einem idealen Gas aus Atomen der Massen $m > 0$ ($m < M$). Das Brownsche Teilchen soll sich nur im Intervall $\Lambda \subset \mathbb{R}$ aufhalten können (mit elastischen Reflexionen am Rand), wobei die Ränder des Intervalls für die Gasteilchen durchlässig sind, so dass die Atome durch die Wände in keinsten Weise beeinflusst werden. Da nun der Ort des Brownschen Teilchens beschränkt ist, konvergiert der Prozess des Ortes in der diffusiven Skalierung gegen null. Daher wird ein Prozess R_t konstruiert, der unbeschränkt ist und gewissermaßen die Distanz misst, die das Molekül zurücklegen würde, wäre es nicht im Intervall gefangen. Ziel ist es, für den diffusiv skalierten Prozess R_t diffusives Verhalten zu zeigen. Um dies zu beweisen, zeigen wir, dass der Geschwindigkeitsprozess von R_t die Voraussetzungen des funktionalen Zentralen Grenzwertsatzes (fCLT) von [Dav68], [McL75] erfüllt. Eine wichtige Forderung des fCLTs ist, dass der Geschwindigkeitsprozess α -mischend ist. Zeigt man diese Eigenschaft für einen Markov Prozess, der den Geschwindigkeitsprozess enthält, „erbt“ letzterer diese Eigenschaft. In unserem Fall beschreibt der Markov Prozess im Wesentlichen die Orte und Geschwindigkeiten aller Teilchen in Λ .

Die Positivität der Diffusionskonstanten zeigen wir mit Hilfe eines Resultats von [DG86].

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Eidesstattliche Versicherung

(Siehe Promotionsordnung vom 12.07.2011, §8, Abs. 2 Pkt. 5.)

Hiermit erkläre ich an Eidesstatt, dass die Dissertation von mir selbstständig, ohne unerlaubte Beihilfe angefertigt ist.

Anneliese Froemel
München, 22. Juli 2020

1 Introduction

Consider the following classical system - a model for a simple non-equilibrium situation in statistical mechanics: Point particles of mass $m > 0$ (atoms) are distributed on the real line according to a Poisson distribution and each atom is initially given a random velocity independent of its position and the other atoms, where we may think of the velocity distribution as being Maxwellian. The atoms interact via elastic collision with a point particle of mass $M > 0$, hereinafter referred as the molecule, whose motion we wish to observe. Let $Q(t)$ denote its position at time t . If the molecule is placed at time zero at the origin, i.e. $Q(0) = 0$, $Q_t = \{Q(t)\}_{t \in \mathbb{R}^+}$ is a stochastic process on the probability space of the random initial conditions of the atoms and the initial velocity of the molecule.

A difficult and in general still unsolved problem is then to prove the following conjecture: For any $T < \infty$, the process

$$Q_{A,t} := \left\{ \frac{1}{\sqrt{A}} Q(At) \right\}_{t \in [0, T]}$$

converges in distribution to the Wiener process

$$\sqrt{D}W_t$$

with diffusion constant

$$D = 2 \int_0^\infty \mathbb{E}(V(t)V(0))dt$$

as $A \rightarrow \infty$, where $V(t)$ denotes the velocity of the molecule at time t and $\mathbb{E}(\cdot)$ denotes the expectation w.r.t. the equilibrium measure of the system. For the definition of a Wiener process see e.g. [Bre68].

This conjecture has been proved for the special case $M = m$ by [Spi69]. Spitzer used methods which essentially rely on the equal mass of molecule and atoms and which were previously employed by [Har65] to prove that the finite dimensional distributions of the process $Q_{A,t}$ converge as $A \rightarrow \infty$ to those of a Gaussian process. Further results concerning diffusive behavior of the molecule in the model described above all have in common that they use normalizations where the mass of the molecule or of the atoms tend to infinity resp. to zero with an appropriate speed. [ST87] and [ET92] give a good overview of the results of the 80's and early 90's, when the most work was done on this topic. There are some more actual results like [BTT07], [KL10], [Lia14], where the normalization again depends on the masses.

The motivation for the work described here, was to use methods which do not depend on the choice of the masses for proving the conjecture.

For simplicity let us assume that $V_t = \{V(t)\}_{t \in \mathbb{R}^+}$ is a stationary process and let us write

$$Q_A(t) = \frac{1}{\sqrt{A}} \int_0^{At} V(s) ds. \quad (1.1)$$

Here it becomes more evident that we conjecture that $Q_{A,t}$ satisfies an invariance principle (or a functional Central Limit Theorem (fCLT)). Since the molecule can recollide over arbitrary long times with atoms it has previously collided with, the r.h.s. of (1.1) cannot be written as a sum over independent increments. Thus, if a fCLT applies, it necessary will be one for dependent variables. Apart from the problem of finding an appropriate version of a fCLT for dependent variables, one then need to check whether the velocity process V_t fulfills the conditions under which the fCLT holds.

The purpose of this thesis is to explore this possible approach by studying a much simpler model: To gain better control over the recollisions, we consider the molecule to be confined in the interval $\Lambda = [-L, L]$, $L > 0$, with walls at $-L$ and L . Hence, any recollision takes place in Λ . The atoms remain unaffected by the walls, but the walls elastically reflect the molecule. The ergodic properties of such a system are studied in [GLR82] in one dimension and in [ET90] in multidimensions, where in particular it is shown that the molecule approaches its equilibrium state starting from almost all (w.r.t. Lebesgue measure) initial values Q, V .

Mind that in this model $|Q(t)| < L$, i.e. the scaling in (1.1) gives $\frac{1}{\sqrt{A}}Q(At) \rightarrow 0$ as $A \rightarrow \infty$. Therefore, one has to define a new quantity which is unbounded and which can be interpreted as the distance the molecule would have travelled if it wasn't confined in the interval. In [ET92] the quantity

$$Q(t) := \int_0^t |V(s)| ds \quad (1.2)$$

was investigated and diffusive behavior for (1.2) in the usual scaling was shown for $M > m$. In the presented work we define a different quantity $R(t)$ hoping to obtain a fCLT for $M \geq m$. It turns out that we can prove a fCLT for $M > m$. However, these methods fail for $M = m$.

One goal of the thesis is to give an explicit bound for the rate of dependency, which allows to analyze the bound for $M \rightarrow m$ and $L \rightarrow \infty$. As discussed before, confining the molecule to the finite region $[-L, L]$ gives control over recollisions. It turns out that our model does not allow to remove the cut off in the recollisions to obtain the unrestricted motion, i.e. we cannot proceed from the theorem proven here to the conjecture.

In the next chapter, Chapter 2, we describe the model in detail and give the main result. In Chapter 3 we introduce a notion of weak dependence of random variables in the form of α -mixing and state a general fCLT. In Chapter 4, Chapter 5 and Chapter 6 we show

that the conditions of the fCLT are satisfied by our model, thereby proving the result. In doing so we deepen also the results of [GLR82] in that we obtain estimates on the rates of convergence to equilibrium in the sense of β -mixing. In the last two chapters, Chapter 7 and Chapter 8, we discuss our results and give some ideas for future research projects.

For reasons of clarity, we now name the crucial theorems and propositions proven in Chapter 5 and Chapter 6.

Our main result is formulated in Theorem 2.1, which we prove by a fCLT (Theorem 3.1). There are mainly two conditions in the fCLT which have to be proved for our model to obtain Theorem 2.1. These follow by Proposition 5.1 (see Chapter 5) and by Proposition 6.1 (see Chapter 6).

The crucial Lemma in Chapter 5 for showing Proposition 5.1 is the Overlap-Lemma 5.2. To prove this, we give Lemma 5.4, Lemma 5.5, Lemma 5.6 and the overlap size in Lemma 5.7; these together give Lemma 5.8. The Overlap-Lemma follows then by Lemma 5.3 and Lemma 5.8. By Corollary 5.1 and Corollary 5.2, which are implications of the Overlap-Lemma 5.2, and by Lemma 5.9 we obtain finally Proposition 5.1.

Proposition 6.1 in Chapter 6 follows by Lemma 6.7. The crucial lemmata for proving Lemma 6.7 are Lemma 6.1 (which is proved by several assertions) with its implication Corollary 6.1, as well as Lemma 6.2 and Lemma 6.3. The latter follows by Lemma 6.4, Lemma 6.5 and Lemma 6.6.

2 The model and the main result

Consider the following infinite particle system in one dimension. The underlying dynamics is governed by classical mechanics. A point particle with mass $M > 0$ (“molecule”) moves in the interval $\Lambda = [-L, L] \subset \mathbb{R}$, $L > 0$. It is in contact with an ideal gas of point particles of mass $m > 0$ (“atoms”), which are distributed on the real line. The atoms interact with the molecule via elastic collisions, but do not interact with each other. Let q, v denote the position and velocity of the atoms, while Q, V denote the position and velocity of the molecule. The post collision velocities V', v' are determined by energy and momentum conservation which lead to the following equations.

$$V' = \frac{M - m}{M + m}V + \frac{2m}{M + m}v, \quad (2.1)$$

$$v' = -\frac{M - m}{M + m}v + \frac{2M}{M + m}V. \quad (2.2)$$

Between the collisions all particles move with constant velocity. Let $Q(t), V(t)$ denote the position and velocity of the molecule at time t . At the walls $-L$ and L the molecule is reflected elastically, i.e. the velocity is reversed with

$$V(\tau) = -V(\tau_-)$$

where $\tau \in \{t \in \mathbb{R}^+ : Q(t) \in \{-L, L\}\}$ is a reflection time and τ_- denotes the time right before the molecule is reflected by one of the walls. The walls are permeable for the atoms. Let

$$\hat{\Omega} = \Lambda \times \mathbb{R} \times \Omega \quad (2.3)$$

denote the phase space of the system with σ -algebra \mathcal{F} , where $\Omega = \mathbb{R}^{2\mathbb{N}}$ is the phase space of the ideal gas. For $\hat{\omega} \in \hat{\Omega}$ we have $\hat{\omega} = ((Q, V), X)$, where $(Q, V) \in \Lambda \times \mathbb{R}$ and $X \in \Omega$ stands for the configuration of the ideal gas particles, i.e. $X = (q_n, v_n)_{n \in \mathbb{N}}$, $q_n \in \mathbb{R}, v_n \in \mathbb{R}$. The stationary measure for the evolution of the system is the infinite volume Gibbs state at some temperature $T > 0$ and gas density $\rho > 0$. We denote this measure by μ . Then, the ideal gas is distributed in phase space according to the Poisson distribution \mathcal{P} with the one-particle phase space measure ν given by

$$d\nu = \rho f(v)dvdq, \quad (2.4)$$

where $dvdq$ denotes the Lebesgue measure on \mathbb{R}^2 and $f(v)$ is the Maxwellian, i.e.

$$\begin{aligned} f : \mathbb{R} &\rightarrow \mathbb{R} \\ v &\mapsto \left(\frac{\mathcal{K}m}{2\pi}\right)^{\frac{1}{2}} e^{-\frac{\mathcal{K}m}{2}v^2}, \end{aligned} \tag{2.5}$$

with $\mathcal{K} = (k_B T)^{-1}$ and where k_B is the Boltzmann constant. Hence, for measurable $A \subset \mathbb{R}^2$ we have that the number of atoms in A is a random variable \mathcal{N}_A with distribution

$$\mathcal{P}(\mathcal{N}_A = k) = e^{-\nu(A)} \frac{\nu(A)^k}{k!}, \quad k \in \mathbb{N}_0 \tag{2.6}$$

and for measurable $A, B \subset \mathbb{R}^2$

$$A \cap B = \emptyset \Rightarrow \mathcal{N}_A \text{ and } \mathcal{N}_B \text{ are independent.} \tag{2.7}$$

The distribution of the position and velocity of the molecule is

$$\mu_M(dQ, dV) := \left(\frac{\mathcal{K}M}{2\pi}\right)^{\frac{1}{2}} e^{-\frac{\mathcal{K}}{2}MV^2} dV \frac{1}{2L} dQ, \tag{2.8}$$

since $Q \in \Lambda$. The stationary measure μ of the system is given by

$$\mu((dQ, dV), dX) = \mu_M(dQ, dV) \times \mathcal{P}(dX). \tag{2.9}$$

Note that μ is finite, since \mathcal{P} is normalized and the molecule is confined in Λ .

Denote by Φ_t the time evolution of this system. For $\hat{\omega} \in \hat{\Omega}$, $\Phi_t(\hat{\omega})$ is the phase space point (configuration) to which $\hat{\omega}$ evolves in time t^1 , i.e.

$$\begin{aligned} \Phi_t : \hat{\Omega} &\rightarrow \hat{\Omega} \\ \hat{\omega} &\mapsto ((Q(\hat{\omega}, t), V(\hat{\omega}, t)), X(\hat{\omega}, t)), \end{aligned} \tag{2.10}$$

where $Q(\cdot, t), V(\cdot, t), X(\cdot, t)$ are random variables on $(\hat{\Omega}, \mathcal{F}, \mu)$. In the following we will write $Q(t)$ instead of $Q(\hat{\omega}, t)$ (etc.) whenever it is unambiguous.

As discussed in Chapter 1, we introduce the random variable $R(t)$, which is unbounded and which in some appropriate sense measures the distance the molecule would travel without confinement. To define $R(t)$ we use an extra random function $\sigma(t)$ which is defined on a trivially enlarged sample space $\hat{\Omega} \times \{-1, 1\}$, and we obtain the probability space

$$\Sigma := (\hat{\Omega} \times \{-1, 1\}, \mathcal{F} \times \mathcal{P}(\{-1, 1\}), \mu \times \rho), \tag{2.11}$$

¹The time evolution is almost surely w.r.t. the stationary measure (defined in (2.9)) well defined, i.e. multiple simultaneous collisions and infinitely many collisions in a finite amount of time are atypical. For a proof in a very similar system see for example [GLR82].

where \mathcal{P} denotes the power set and ρ is a discrete measure, which weights the initial value $\sigma(0)$. We set

$$R(t) := \int_0^t U(s) ds \quad (2.12)$$

where

$$U(t) := \sigma(t)V(t) \quad (2.13)$$

is a random variable on Σ (cf. (2.11)) and $\sigma(t)$ is defined now as follows. Let $P(t) = (P_x(t), P_y(t))$ denote the point on a circle of radius L centered in the origin. Note that the x -axis is the real line on which the motion takes place. Let

$$P_x(t) = Q(t)$$

and we define

$$\sigma(t) := \text{sign}(P_y(t)), \quad (2.14)$$

whereby the y -coordinate $P_y(t)$ shall change sign whenever $Q \in \{-L, L\}$. Moreover, for all $t \in \mathbb{R}$ $Q(t) \in \{-L, L\}$, $\sigma(t) = +1$ means that $P(t)$ moves in positive y direction and $\sigma(t) = -1$ means $P(t)$ moves in negative direction.

Hence, $R(t)$ only changes direction due to the collisions with atoms and not because of the presence of the walls. $R(t)$ can be seen as the distance the molecule would move without confinement. We find $R(t) \in \mathbb{R}$.

Note, for given $\sigma(0)$, $\{\sigma(t)\}_{t>0}$ is a stochastic process on $(\hat{\Omega}, \mathcal{F}, \mu)$.

Let

$$U_t := \{U(t)\}_{t \in \mathbb{R}^+} \quad (2.15)$$

be the stochastic process defined on Σ (cf. (2.11)) with $U(t)$ given in (2.13). Denote by $\rho_{\frac{1}{2}}$ the discrete measure with

$$\rho_{\frac{1}{2}}(\sigma) = \frac{1}{2}, \sigma \in \{-1, 1\}. \quad (2.16)$$

We show in Chapter 4 that choosing

$$\rho = \rho_{\frac{1}{2}}$$

in Σ (cf. (2.11)) U_t is a stationary process, and we define

$$\Sigma_{\frac{1}{2}} := \left(\hat{\Omega} \times \{-1, 1\}, \mathcal{F} \times \mathcal{P}(\{-1, 1\}), \mu \times \rho_{\frac{1}{2}} \right) \quad (2.17)$$

with μ given in (2.9) and $\rho_{\frac{1}{2}}$ given in (2.16).
 To state our main result define for any $A > 0$

$$R_A(t) := \frac{1}{\sqrt{A}}R(At) \stackrel{(2.12)}{=} \frac{1}{\sqrt{A}} \int_0^{At} U(s)ds.$$

Then,

$$R_{A,t} := \{R_A(t)\}_{t \in \mathbb{R}^+} \tag{2.18}$$

is by definition a continuous process. Let $I = [0, T]$ for some $0 < T < \infty$. By \mathcal{R}_A we denote the path measure generated by the process $R_{A,t}$ on $C(I)$, the space of the continuous functions on I , equipped with the uniform topology. Let \mathcal{W}_D denote the Wiener measure with diffusion constant D . For the definition of the Wiener measure see [Bil99].

Our main result is:

Theorem 2.1. Let $M > m > 0$. Consider the stochastic process $R_{A,t}$ as defined in (2.18) and $U(t)$ as given in (2.13) on $\Sigma_{\frac{1}{2}}$ (cf. (2.17)).

Then,

$$0 < D = 2 \int_0^\infty \mathbb{E}(U(0)U(t))dt < \infty, \tag{2.19}$$

where $\mathbb{E}(\cdot)$ denotes the expectation w.r.t. $\mu \times \rho_{\frac{1}{2}}$ (cf. (2.17)), and for any $0 < T < \infty$

$$\{R_A(t)\}_{t \in [0, T]} \Rightarrow \sqrt{D}W_{t \in [0, T]}, \text{ as } A \rightarrow \infty$$

in the sense of weak convergence of the measures \mathcal{R}_A to \mathcal{W}_D defined on $C([0, T])$.

For the notation of weak convergence see [Bil99].

3 A functional Central Limit Theorem

To prove our main result (Theorem 2.1), we use a fCLT which is originated in [Dav68] and was improved by [McL75]. To show the positivity of the diffusion constant D (cf. (2.19)) we use a result of [DG86]. To state the fCLT, we need to introduce the notion of α -mixing. Let $X_t = \{X(t)\}_{t \in \mathbb{R}^+}$ be a stationary sequence of random variables on the probability space (Ω, \mathcal{F}, P) . Denote by

$$\mathcal{F}_{s,t}^X := \sigma(X(u), s \leq u \leq t)$$

the σ -algebra generated by $\{X(u), s \leq u \leq t\}$ and let

$$\alpha_X(t) := \alpha(\mathcal{F}_{-\infty,0}^X, \mathcal{F}_{t,\infty}^X) := \sup_{A \in \mathcal{F}_{-\infty,0}^X, B \in \mathcal{F}_{t,\infty}^X} |P(AB) - P(A)P(B)|. \quad (3.1)$$

X_t is called *α -mixing* (or *strong mixing*) if $\alpha_X(t) \rightarrow 0$ with $t \rightarrow \infty$. Note that “mixing in the ergodic-theoretic sense” is weaker than α -mixing (see e.g. [Bra05]).

We now state the fCLT of [Dav68] (Theorem 5.2) and [McL75] (Corollary 3.9) supplemented by a result of [DG86] (Corollary 3.17).

Theorem 3.1. Let $(X_t, \Omega, \mathcal{F}, \mathbb{P})$ be a stationary process with

$$\mathbb{E}(X(0)) = 0 \quad (3.2)$$

and

$$0 < \mathbb{E}(X(0)^2) < \infty. \quad (3.3)$$

Suppose there exists $\delta > 0$ such that

$$\mathbb{E}(|X(0)|^{2+\delta}) < \infty, \quad (3.4)$$

and that X_t is α -mixing with

$$\int_0^\infty \alpha_X(t)^{\frac{\delta}{2+\delta}} dt < \infty, \quad (3.5)$$

then

$$D = 2 \int_0^\infty \mathbb{E}(X(0)X(t))dt < \infty$$

and

$$\{S_A(t)\}_{t \in [0,1]} := \left\{ \frac{1}{\sqrt{A}} \int_0^{At} X(s)ds \right\}_{t \in [0,1]} \Rightarrow \{\sqrt{D}W(t)\}_{t \in [0,1]}, \text{ as } A \rightarrow \infty$$

in the sense that \mathcal{S}_A , the measure on $C([0, 1])$ generated by $S_{A,t} := \{S_A(t)\}_{t \in [0,1]}$, converges weakly to the Wiener measure \mathcal{W}_D^1 .

Furthermore, if

$$\sup_t \mathbb{E}(|S_1(t)|) = \sup_t \mathbb{E} \left(\left| \int_0^t X(s)ds \right| \right) = \infty, \quad (3.6)$$

where \mathbb{E} is the expectation w.r.t. the measure \mathbb{P} , it follows from Corollary (3.17) in [DG86] that

$$D > 0.$$

See [Pel86] or [Dou94] for a good survey about sufficient and necessary conditions for (f)CLTs for mixing sequences.

To prove our main result (Theorem 2.1), we show that the process U_t (cf. (2.15)) defined on $\Sigma_{\frac{1}{2}}$ (cf. (2.17)) fulfills the conditions of the fCLT (Theorem 3.1). In the next chapter we prove that the process U_t on (2.17) is stationary w.r.t. the measure $\mu \times \rho_{\frac{1}{2}}$ (cf. (2.17)) and consequently $\mathbb{E}(U(0)) = 0$, $0 < \mathbb{E}(U(0)^2) < \infty$ as well as Condition (3.4) is fulfilled for any $\delta > 0$. In Chapter 5 we show that the stationary process U_t is α -mixing with (3.5) for some $\delta > 0$, and in Chapter 6, we will prove that U_t satisfies Condition (3.6).

¹If $D = 0$, $S_{A,t}$ converges in distribution to the zero-function as $A \rightarrow \infty$.

4 A stationary distribution of the stochastic process U_t

In this chapter, we show that the stochastic process U_t (cf. (2.15)) is stationary w.r.t. the measure $\mu \times \rho_{\frac{1}{2}}$ (cf. (2.17)). The stationarity of U_t is one of the requirements of the fCLT (Theorem 3.1) from which we obtain our main result.

Lemma 4.1. Consider the stochastic process U_t as given in (2.15) defined on $\Sigma_{\frac{1}{2}}$ (cf. (2.17)). Then, U_t is a stationary stochastic process.

Proof of Lemma 4.1. To prove Lemma 4.1 we make use of the *Skew-Product-Lemma* [Pet83]:

Lemma 4.2 (*Skew-Product-Lemma*). Let ρ_t be a measure preserving map on the measure space (\mathcal{X}, ξ) , with state space \mathcal{X} and measure ξ , and let for $x \in \mathcal{X}$ h_t^x be a map on (\mathcal{Y}, θ) such that h_t^x preserves θ . Denote by (\mathcal{Z}, ν) the direct product measure space of (\mathcal{X}, ξ) and (\mathcal{Y}, θ) , i.e.

$$\mathcal{Z} = \mathcal{X} \times \mathcal{Y}, \quad z = (x, y), \quad x \in \mathcal{X}, y \in \mathcal{Y}$$

and

$$\nu = \xi \times \theta.$$

Then, the evolution

$$\Psi_t(x, y) = (\rho_t(x), h_t^x(y))$$

is a measure preserving function on (\mathcal{Z}, ν) .

We apply the *Skew-Product-Lemma* 4.2 to the following situation. We consider \mathcal{X} to be the phase space of the system of all particles (ideal gas and the molecule), i.e.

$$\mathcal{X} = \hat{\Omega}$$

(cf. (2.3)). The measure ξ is then the product of ideal gas measure with Gibbs measure of the molecule, i.e.

$$\xi = \mu$$

(cf. (2.9)). Let

$$\mathcal{Y} = \{-1, 1\}.$$

We consider the evolution

$$\tilde{\Phi}_t(\hat{\omega}, \sigma) := (\Phi_t(\hat{\omega}), \kappa_t^{\hat{\omega}}(\sigma)) \quad (4.1)$$

on $\mathcal{X} \times \mathcal{Y}$ where Φ_t is the dynamical evolution of the system of all particles (cf. (2.10)), and

$$\begin{aligned} \kappa_t^{\hat{\omega}} : \{-1, 1\} &\rightarrow \{-1, 1\} \\ \sigma(0) &\mapsto \sigma(t). \end{aligned}$$

Now we show that $\kappa_t^{\hat{\omega}}$ preserves $\rho_{\frac{1}{2}}$, i.e. that for any $B \in \mathcal{P}(\{-1, 1\})$

$$\rho_{\frac{1}{2}}((\kappa_t^{\hat{\omega}})^{-1}(B)) = \rho_{\frac{1}{2}}(B).$$

Let

$$A_{\text{even}} := \{\text{The molecule is reflected an even number of times during } [0, t]\} \subset \hat{\Omega}$$

$$A_{\text{odd}} := \{\text{The molecule is reflected an odd number of times during } [0, t]\} \subset \hat{\Omega}.$$

Note that $A_{\text{even}} \cap A_{\text{odd}} = \emptyset$ and $A_{\text{even}} \cup A_{\text{odd}} = \hat{\Omega}$. For $\sigma \in \{-1, 1\}$ and $\hat{\omega} \in A_{\text{even}}$ we have that

$$(\kappa_t^{\hat{\omega}})^{-1}(\sigma) = \sigma, \quad (4.2)$$

and for $\hat{\omega} \in A_{\text{odd}}$ that

$$(\kappa_t^{\hat{\omega}})^{-1}(\sigma) = -\sigma. \quad (4.3)$$

Then, we obtain for $\sigma \in \{-1, 1\}$ and $\hat{\omega} \in A_{\text{even}}$ that

$$\rho_{\frac{1}{2}}((\kappa_t^{\hat{\omega}})^{-1}(\sigma)) \stackrel{(4.2)}{=} \rho_{\frac{1}{2}}(\sigma)$$

and for $\hat{\omega} \in A_{\text{odd}}$

$$\rho_{\frac{1}{2}}((\kappa_{1,t}^{\hat{\omega}})^{-1}(\sigma)) \stackrel{(4.3)}{=} \rho_{\frac{1}{2}}(-\sigma) = \rho_{\frac{1}{2}}(\sigma).$$

Thus, $\kappa_t^{\hat{\omega}}$ preserves $\rho_{\frac{1}{2}}$.
 Considering

$$\theta = \rho_{\frac{1}{2}},$$

we obtain by the *Skew-Product-Lemma* that $\tilde{\Phi}_t$ (cf. (4.1)) is a measure preserving function on

$$\Sigma_{\frac{1}{2}} \stackrel{(2.11)}{=} \left(\hat{\Omega} \times \{-1, 1\}, \mathcal{F} \times \mathcal{P}(\{-1, 1\}), \mu \times \rho_{\frac{1}{2}} \right).$$

Since $U(t)$ (cf. (2.13)) is a function of $\tilde{\Phi}_t$, Lemma 4.1 follows. \square

From now on denote by U_t the stationary process

$$\left(U_t, \hat{\Omega} \times \{-1, 1\}, \mathcal{F} \times \mathcal{P}(\{-1, 1\}), \mu \times \rho_{\frac{1}{2}} \right). \quad (4.4)$$

Then, U_t fulfills Condition (3.2) and Condition (3.3) of the fCLT (Theorem 3.1), since $V(0)$ and $\sigma(0)$ are independent, and since by Lemma 4.1 $V(0)$ is distributed according to the Maxwellian given in (2.8) and $\sigma(0)$ is distributed according to $\rho_{\frac{1}{2}}$ (cf. (2.16)). We have that

$$\mathbb{E}(U(0)) \stackrel{(2.13)}{=} \mathbb{E}(\sigma(0)V(0)) = \mathbb{E}(\sigma(0))\mathbb{E}(V(0)) = 0$$

and

$$0 < \mathbb{E}(U(0)^2) \stackrel{(2.13)}{=} \mathbb{E}(\sigma(0)^2)\mathbb{E}(V(0)^2) < \infty. \quad (4.5)$$

(4.5) follows, since it is well known that for a random variable which is distributed according to the Maxwellian all moments of arbitrary order exist. By this argument and as a consequence of the independency of $V(0)$ and $\sigma(0)$ all moments of arbitrary order of $U(0)$ exist, such that Condition (3.4) is fulfilled for any $\delta > 0$.

5 U_t is rapidly α -mixing

In this chapter, we prove that U_t is α -mixing with (3.5) for some $\delta > 0$. First, we give the general idea of the proof by introducing a stronger form of mixing (β -mixing), followed by the presentation of the proof.

5.1 General idea of the proof

Consider the stationary process U_t as given in (4.4). To show our main result (Theorem 2.1), by the fCLT (Theorem 3.1) we have to prove that U_t is rapidly α -mixing. By that we mean, U_t is α -mixing and Condition (3.5) is satisfied.

Establishing rapid α -mixing is in general a difficult task, except if U_t is a function on the state space of a stationary *good Harris mixing* Markov process (see [DGL83]): Let $\mathcal{M}_t = \{\mathcal{M}(t)\}_{t \in \mathbb{R}^+}$ be a Markov process with state space $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$, transition probability Π_x^t , $x \in \mathcal{X}$ and stationary measure Π , i.e. $\Pi(\cdot) = \int \Pi(dx) \Pi_x^t(\cdot)$. If $U(t)$ is a function of $\mathcal{M}(t)$, then for any $s, v \in \mathbb{R}^+$

$$\sigma(U(t), s \leq t \leq v) \subset \sigma(\mathcal{M}(t), s \leq t \leq v)$$

and by the definition of $\alpha_X(t)$ (cf. (3.1)) it follows that

$$\alpha_U(t) \leq \alpha_{\mathcal{M}}(t). \tag{5.1}$$

Hence, the process U_t inherits the property of α -mixing of the Markov process \mathcal{M}_t . Furthermore, the Markov process \mathcal{M}_t is rapidly α -mixing if it is *good Harris mixing*. To define the property of Harris mixing, we introduce the total variation distance. Let μ, ν be probability measures defined on the same measurable space (Ω, \mathcal{F}) . Then, the *total variation distance* of μ and ν is defined by

$$\|\mu - \nu\| := 2 \sup_{A \in \mathcal{F}} |\mu(A) - \nu(A)|.$$

Note that for probability measures

$$\|\mu - \nu\| \leq 2. \tag{5.2}$$

The stationary process \mathcal{M}_t is called *Harris mixing* if for Π a.e. x

$$\|\Pi_x^t - \Pi\| \rightarrow 0, \text{ for } t \rightarrow \infty.$$

From the Markov property it follows that

$$\alpha_{\mathcal{M}}(t) \leq \int \Pi(dx) \|\Pi_x^t - \Pi\|. \quad (5.3)$$

The r.h.s. of (5.3) is known as the β -coefficient for stationary Markov processes. For a stationary Markov process X_t with transition Π_x^t and stationary measure Π , we write

$$\beta_X(t) := \int \Pi(dx) \|\Pi_x^t - \Pi\|. \quad (5.4)$$

If

$$\beta_X(t) \rightarrow 0, \text{ as } t \rightarrow \infty$$

the process X_t is called β -mixing (or *absolute regular*) (see e.g. [Dav73] or [Dou94] for a good survey about β -mixing).

Since by (5.1) and (5.3) it follows that

$$\alpha_U(t) \leq \beta_{\mathcal{M}}(t),$$

we obtain rapid α -mixing of the process U_t by rapid β -mixing (or: by *good Harris mixing*) of the stationary process \mathcal{M}_t .

Some remarks on the β -coefficient

The property of β -mixing of a process expresses, as any mixing does, that for large enough separation of future and past, the evolution of the process become independent. To see that, we follow [Dou94] to provide a more intuitive definition of the β -coefficient for a stationary (not necessary Markov) process $(X_t, \Omega, \mathcal{F}, \mathbb{P})$. Let $\mathbb{P}|_{\mathcal{F}}$ denote the measure restricted to the σ -algebra \mathcal{F} , and we write

$$\mathbb{P}_0 := \mathbb{P}|_{\mathcal{F}_{-\infty,0}^X},$$

$$\mathbb{P}^t := \mathbb{P}|_{\mathcal{F}_{t,\infty}^X}.$$

Let $\mathbb{P}_{0,t}$ denote the conditional measure on \mathcal{F}_t^∞ given $\mathcal{F}_{-\infty}^0$. Then, one defines

$$\beta_X(t) := \|\mathbb{P}_0 \mathbb{P}_{0,t} - \mathbb{P}_0 \times \mathbb{P}^t\|. \quad (5.5)$$

Note that if X_t is Markov, Definition (5.4) and Definition (5.5) are equivalent (see [Dou94] and [Dav73]). It becomes clearer now that β quantifies the degree of dependence of the past and the future of the process: Roughly speaking, $\mathbb{P}_0 \times \mathbb{P}^t$ would be the measure which arises if $\{X(s), s \leq 0\}$ and $\{X(s), s \geq t\}, t > 0$ were independent, whereas $\mathbb{P}_0 \mathbb{P}_{0,t}$ is the true measure for events $C \in \mathcal{F}_{-\infty,0}^X \times \mathcal{F}_{t,\infty}^X$.

To be precise, $\frac{2-\beta_X(t)}{2}$ measures the *overlap* of $\mathbb{P}_0 \times \mathbb{P}^t$ and $\mathbb{P}_0 \mathbb{P}_{0,t}$: Two measures μ and ν

on the same measurable space (Ω, \mathcal{F}) are *overlapping* if μ and ν are not mutually singular, i.e. for any $A, B \in \mathcal{F}$

$$(\mu(A) = 1) \wedge (\nu(B) = 1) \Rightarrow A \cap B \neq \emptyset.$$

Note that μ has an absolutely continuous component with respect to ν if and only if μ and ν are overlapping ([GLR82]). Using an equivalent definition of the total variation distance, namely

$$\|\mu - \nu\| = 2 - 2(\mu \wedge \nu)(\Omega)$$

where

$$(\mu \wedge \nu)(A) := \int_A \min\{D_\mu(\omega), D_\nu(\omega)\}(\mu + \nu)(d\omega)$$

and $D_\mu(\omega)$, $D_\nu(\omega)$ denote the Radon-Nikodym-derivatives with respect to $(\mu + \nu)$, it is quite intuitive that one may quantify the overlap of two measures μ and ν by

$$(\mu \wedge \nu)(\Omega) = \frac{2 - \|\mu - \nu\|}{2}.$$

Having (5.4) in mind, it becomes clear that with

$$\beta_X(t) = \int \Pi(dx) \|\Pi_x^t - \Pi\| \leq \int \Pi(dx) \int \Pi(dx') \|\Pi_x^t - \Pi_{x'}^t\|$$

an appropriate control over the overlap of the transition probabilities Π_x^t , $\Pi_{x'}^t$ when varying over t and x, x' , gives a good mixing rate, since then $\|\Pi_x^t - \Pi_{x'}^t\|$ decays fast enough (see [DGL83]).

5.2 Proof: U_t is rapidly α -mixing

According to the statements made in the previous section, α -mixing of U_t (cf. (4.4)) follows as soon as we show β -mixing for a stationary Markov process which contains U_t . Due to the confinement of the molecule to Λ , there exists a “natural” Markov process \mathcal{M}_t which is intermediate between the non-Markovian process U_t and the deterministic evolution of the infinite dynamical system (see [GLR82]). Let $Y(t)$ be the configuration of all particles in Λ and the value of σ at time t . Let $q_i(t), v_i(t), i \in \mathbb{N}$, denote the positions and velocities of the atoms which are in Λ at time t , then

$$Y(t) = (Q(t), V(t), q_i(t), v_i(t), \sigma(t)). \quad (5.6)$$

We define the process

$$\mathcal{M}_t := \{Y(t)\}_{t \in \mathbb{R}^+} \quad (5.7)$$

on $\Sigma_{\frac{1}{2}}$ (cf. (2.17)) with state space $\hat{\Omega}|_{\Lambda} \times \{-1, 1\}$, where $\hat{\Omega}|_{\Lambda}$ is the set of all configurations in Λ . To show that the process thus defined is indeed well defined in the sense of being measurable, we refer the reader to a rather general result of [KL10] where measurability of collision processes was established.

We now show that \mathcal{M}_t is a stationary Markov process.

Lemma 5.1. The process \mathcal{M}_t defined in (5.7) is Markov and stationary w.r.t. the measure

$$\Pi(dy) = \mu \times \rho_{\frac{1}{2}}(Y(0) \in dy), \quad (5.8)$$

where $\mu \times \rho_{\frac{1}{2}}$ is given in (4.4).

Proof of Lemma 5.1. We first show the Markov property of \mathcal{M}_t . Let $\tau > 0$. The knowledge of $\{Y(t)\}_{t \leq \tau}$ is equivalent to the knowledge of $Y(\tau)$ and of all atoms, which have left Λ until τ , since apart from the incoming atoms the evolution of $\sigma(t)$ is deterministic. The evolution after time τ is determined by $Y(\tau)$ and the atoms which enter the interval after τ . This follows inter alia from the fact that given $\sigma(\tau)$, $\{\sigma(t), t > \tau\}$ is determined by $Y(\tau)$ and all atoms entering Λ after time τ . Since an atom which enters Λ after τ is dynamically independent of the evolution of the process before τ (an atom which leaves the interval, never returns, i.e. atoms which enter the interval are “fresh”), the Markov property of \mathcal{M}_t follows.

Since $Y(t)$ is a function of $\tilde{\Phi}_t$ (cf. (4.1)), \mathcal{M}_t inherits its stationary distribution from $\mu \times \rho_{\frac{1}{2}}$, i.e.

$$\Pi(dy) = \mu \times \rho_{\frac{1}{2}}(Y(0) \in dy).$$

□

As we pointed out in Section 5.1, rapid α -mixing of the process U_t (Condition (3.5) of the fCLT (Theorem 3.1)) follows if $\mathcal{M}_t = \{Y(t)\}_{t \in \mathbb{R}^+}$ is rapid β -mixing, since $U(t)$ (cf. (2.13)) is a function of $Y(t)$ (cf. (5.6)), i.e. Condition (3.5) follows as soon as we show following proposition.

Proposition 5.1. Consider the process \mathcal{M}_t as defined in (5.7). Then, there exists a $\delta > 0$ such that \mathcal{M}_t is β -mixing with

$$\int_0^\infty \beta_{\mathcal{M}}(t)^{\frac{\delta}{2+\delta}} dt < \infty.$$

Note that we proved in Chapter 4 that Condition (3.4) of the fCLT (Theorem 3.1) is fulfilled for any $\delta > 0$.

Hereinafter, we neglect the index \mathcal{M} on $\beta_{\mathcal{M}}$ and write only β . The idea of proving Proposition 5.1 is the following. Having in mind that \mathcal{M}_t is a Markov process with stationary measure Π (cf. (5.8)) such that

$$\beta(t) \stackrel{(5.4)}{=} \int \Pi(dx) \|\Pi_x^t - \Pi\|,$$

we proof overlap of Π_x^τ and Π (transition and stationary measure of \mathcal{M}_t) for x in a “good” set \mathcal{G} (τ is a fixed time and depends on \mathcal{G}). By the existence of an overlap by time τ , one obtains by induction an estimate for $\beta(n\tau)$ which depends on the measure of the overlap and of the measure of \mathcal{G}^c , the complement of \mathcal{G} . Then, we show that \mathcal{G} can be chosen so large that the “bad” set \mathcal{G}^c has very small measure. In fact, we choose \mathcal{G} as depending on n , such that the measure of \mathcal{G}^c approaches zero fast enough as $n \rightarrow \infty$ and such that the overlap doesn't shrink too fast (if \mathcal{G} grows, the overlap becomes small), which gives a good estimate for the β -coefficient.

We begin now by proving first the existence of an overlap set by the following lemma. Denote by Π_y^t the transition probability of \mathcal{M}_t at time t starting in $Y(0) = y \in \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$.

Lemma 5.2. *Overlap-Lemma*

There exist a measurable set $\mathcal{G} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$, a time $t(\mathcal{G})$ and $\gamma(\mathcal{G}) < 2$, which all will be specified later, such that

$$\|\Pi_{y_1}^{t(\mathcal{G})} - \Pi_{y_2}^{t(\mathcal{G})}\| \leq \gamma(\mathcal{G}) \tag{5.9}$$

for any $y_1, y_2 \in \mathcal{G}$.

To show the Overlap-Lemma 5.2, we prove the existence of an overlap set, i.e. loosely speaking a set of states, where any state can be reached at a certain time with probability bounded away from zero if starting in \mathcal{G} . For that we show first that any state in \mathcal{G} can reach a state where the molecule is alone and its velocity is in a certain interval at a certain time (see Lemma 5.6). Having that, we can control the evolution of the process, especially the value of σ , by sending in atoms such that the process may reach at a given time a set of certain states with positive probability (see Lemma 5.7).

This gives us a hint how to choose \mathcal{G} , since there are two kind of states, which could be problematic as starting states: If the molecule is very fast, it may be impossible to slow it down to a given velocity in a given time with a probability large enough. Also many slow atoms in the interval could be a problem, since they may not be kicked out before a given

time with a large enough probability. Therefore, we will choose \mathcal{G} such that these states are excluded i.e. the number of atoms in Λ and their velocity, as well as the velocity of the molecule is bounded.

Since the proof of the Overlap-Lemma 5.2 needs several preliminary lemmata, we first provide these and give the proof of Overlap-Lemma 5.2 afterwards.

Let $0 < \bar{V} < \infty$, $\bar{N} \in \mathbb{N}$ and let

$$G_{\bar{V}, \bar{N}} := \{|v| < \bar{V}, |V| < \bar{V}, N \leq \bar{N}\} \quad (5.10)$$

where $\{|v| < \bar{V}, |V| < \bar{V}, N \leq \bar{N}\} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ denotes the set of configurations for which the molecule and the atoms in Λ have speed less than \bar{V} and the number of atoms in Λ is less or equal \bar{N} . Let B and C be constants with $B < \bar{V}$ and

$$C := \frac{9M^2}{M^2 - m^2} B. \quad (5.11)$$

Recall that M is the mass of the molecule and m the mass of any atom. We first proceed from $G_{\bar{V}, \bar{N}}$ to

$$G_{B,C;0} := \{B < |V| < C, N = 0\} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}, \quad (5.12)$$

which is the set of configurations for which the molecule has speed faster than B but slower than C and is alone in Λ . Since this procedure is rather lengthy, we proceed in several steps.

By the collision equations (2.1) and (2.2) we get following assertion.

Assertion 5.1. Let

$$t_B := \frac{2L}{B}. \quad (5.13)$$

Then, an atom which is in Λ at time t cannot make the molecule faster than B after time $t + t_B$.

Proof of Assertion 5.1. To make the molecule faster than B , the atom has to move towards the molecule and it is necessary (but not sufficient), that $|v| > B$. Let v_t denote the velocity at time t of an atom in Λ . Then,

- (i) if $|v_t| < B$: The atom can only achieve $|v| > B$ by a collision with the molecule. But that leads to a velocity directed in the opposite direction of the molecule. Once an atom moves away from the molecule, it will keep that direction. Hence, the atom

never moves towards the molecule with $|v| > B$, i.e. an atom with $|v_t| < B$ cannot make the molecule faster than B at all.

- (ii) if $|v_t| \geq B$: Let $\tau > t$ denote the first collision time of an atom with the molecule after time t . If $|v_t| \geq B$, then either the atom doesn't collide with the molecule after time t at all or $\tau < t + t_B$. If in the latter case after the collision still $|v| \geq B$, the atom either moves in opposite direction of the molecule and hence cannot make it faster than B anymore, or it moves towards the molecule and collides with it before $t + t_B$ again. As long as the atom has $|v| \geq B$, it will either recollide before $t + t_B$ (if it moves towards the molecule) or it moves in the opposite direction of the molecule and cannot make it faster than B anymore.

Once the atom is slowed down to a speed less than B , it cannot make the molecule faster than B anymore (see (i)).

Thus, if an atom with $|v_t| \geq B$ makes the molecule faster than B , it happens before $t + t_B$.

Taking (i) and (ii) together, Assertion 5.1 follows. □

Consider $Y(0) = y \in G_{\bar{V}, \bar{N}}$. We define the event $\mathcal{E}_{4t_B} \subset \hat{\Omega}$ with

$$\mathcal{E}_{4t_B} = \{\text{No atom enters } \Lambda \text{ during } [0, 4t_B]\} \quad (5.14)$$

The following holds on \mathcal{E}_{4t_B} .

- (a) If $|V(3t_B)| < B$: Since no atom which is at $t = 0$ in Λ , can make the molecule faster than B after t_B (cf. Assertion 5.1), $|V(t)| < B$ for all $t \in [3t_B, 4t_B]$. All atoms with $|v(3t_B)| > B$ must have been slower than B for some time before $3t_B$ (otherwise they would have left the interval by time $2t_B$), and then achieved $|v| > B$ by a collision with the molecule, i.e. these atoms are moving at time $3t_B$ in opposite direction of the molecule and leave Λ by time $4t_B$, without colliding with the molecule, since $|V(t)| < B$ for all $t \in [3t_B, 4t_B]$. Hence, the molecule collides during $[3t_B, 4t_B]$ only with atoms with $|v(3t_B)| < B$. Using (2.2) with pre collision velocities $|V| < B, |v| < B$ gives

$$\begin{aligned} |v'| &= \left| -\frac{M-m}{M+m}v + \frac{2M}{M+m}V \right| \\ &\leq \frac{M-m}{M+m}|v| + \frac{2M}{M+m}|V| \\ &< \frac{M-m}{M+m}B + \frac{2M}{M+m}B \\ &= \frac{3M-m}{M+m}B, \end{aligned} \quad (5.15)$$

i.e. the atoms left in Λ by time $4t_B$ cannot be faster than $\frac{3M-m}{M+m}B$.

- (b) If $|V(3t_B)| > B$: Then, by Assertion 5.1 and by argument (i) in the proof of Assertion 5.1 (taking \bar{V} instead of B), we have that

$$B < |V(t)| < \bar{V}$$

for all $t \in [t_B, 3t_B]$ and all atoms are pushed out of Λ by the molecule by time $3t_B$ i.e. the molecule is alone in Λ by $3t_B$.

With that, the following lemma can be shown.

Lemma 5.3. Consider $G_{B;\bar{N};\tilde{v}}, G_{B,\bar{V};0} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ where we for ease of notation write

$$G_{B;\bar{N};\tilde{v}} := \{ |V| < B, \text{ the number of atoms in } \Lambda \text{ is less or equal } \bar{N}, \text{ the speed of each atom is less than } \tilde{v} := \frac{3M - m}{M + m} B \}, \quad (5.16)$$

$$G_{B,\bar{V};0} := \{ \text{The molecule is alone in } \Lambda \text{ and } B < |V| < \bar{V} \} \quad (5.17)$$

Let t_B be given by (5.13). Then, with

$$C_1 := \frac{1}{2} \exp\left(-\frac{8t_B\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \quad (5.18)$$

we have that for any $y \in G_{\bar{V},\bar{N}}$ either

$$\Pi_y^{4t_B}(G_{B;\bar{N};\tilde{v}}) \geq C_1 \quad (5.19)$$

or

$$\Pi_y^{4t_B}(G_{B,\bar{V};0}) \geq C_1. \quad (5.20)$$

Proof of Lemma 5.3. By facts (a) and (b) from above we have shown that for $Y(0) = y \in G_{\bar{V},\bar{N}}$ it follows that $Y(4t_B) \in G_{B,\bar{V};0} \cup G_{B;\bar{N};\tilde{v}}$ if no atom enters Λ during $[0, 4t_B]$. Hence, for $y \in G_{\bar{V},\bar{N}}$ we have that

$$\Pi_y^{4t_B}(G_{B,\bar{V};0} \cup G_{B;\bar{N};\tilde{v}}) \geq \mu(\mathcal{E}_{4t_B}) \quad (5.21)$$

with \mathcal{E}_{4t_B} given in (5.14).

Denote by $\mathcal{N}(|\Delta|)$ the number of atoms entering Λ during a time interval Δ with length $|\Delta|$, then $\mathcal{N}(|\Delta|)$ is a Poisson random variable with parameter

$$|\Delta|2\rho\left(\sqrt{2\pi\mathcal{K}m}\right)^{-1}, \quad \mathcal{K} \text{ given in (2.5)}$$

i.e.

$$\mu(\{\mathcal{N}(|\Delta|) = k\}) = e^{-|\Delta|2\rho(\sqrt{2\pi\mathcal{K}m})^{-1}} \frac{\left(|\Delta|2\rho(\sqrt{2\pi\mathcal{K}m})^{-1}\right)^k}{k!}, \quad k \in \mathbb{N}_0, \quad (5.22)$$

with

$$\mathbb{E}(\mathcal{N}(|\Delta|)) = |\Delta|2\rho(\sqrt{2\pi\mathcal{K}m})^{-1}.$$

Hence, the probability that no atom enters Λ in a time interval of length $4t_B$ is

$$\mu(\mathcal{E}_{4t_B}) = \exp\left(-\frac{8t_B\rho}{\sqrt{2\pi\mathcal{K}m}}\right). \quad (5.23)$$

Now

$$\Pi_y^{4t_B}(G_{B,\bar{V};0} \cup G_{B,\bar{N};\bar{v}}) \leq 2 \max\left\{\Pi_y^{4t_B}(G_{B,\bar{V};0}), \Pi_y^{4t_B}(G_{B,\bar{N};\bar{v}})\right\}, \quad (5.24)$$

and we obtain Lemma 5.3 since by (5.21) and the estimates (5.23) and (5.24) we obtain that

$$\max\left\{\Pi_y^{4t_B}(G_{B,\bar{V};0}), \Pi_y^{4t_B}(G_{B,\bar{N};\bar{v}})\right\} \geq \frac{1}{2}\mu(\mathcal{E}_{4t_B}) = \frac{1}{2}\exp\left(-\frac{8t_B\rho}{\sqrt{2\pi\mathcal{K}m}}\right) = C_1,$$

i.e. either

$$\Pi_y^{4t_B}(G_{B,\bar{N};\bar{v}}) \geq C_1$$

or

$$\Pi_y^{4t_B}(G_{B,\bar{V};0}) \geq C_1.$$

□

Recall that we want to prove that any state in $G_{\bar{V},\bar{N}}$ (cf. (5.10)) can reach a state in $G_{B,C;0}$ (cf. (5.12)) at a certain time with a certain positive probability. Since we know by Lemma 5.3 that all states in $G_{\bar{V},\bar{N}}$ can either reach $G_{B,\bar{N};\bar{v}}$ (cf. (5.16)) or $G_{B,\bar{V};0}$ (cf. (5.17)) by time $4t_B$, we now proceed from the sets $G_{B,\bar{N};\bar{v}}$ and $G_{B,\bar{V};0}$ to $G_{B,C;0}$ (cf. (5.12)). For that we let atoms enter Λ either to push out the atoms, which are still in Λ or to slow down the molecule.

To handle $G_{B,\bar{N};\bar{v}}$, we use the following assertions. Let

$$D_b := \frac{4M^2}{m(M-m)}B \quad \text{and} \quad D_c := \frac{M+m}{2m}C - \frac{M-m}{2m}B \quad (5.25)$$

with C given in (5.11).

Assertion 5.2. If the molecule with $|V| < B$ collides with an atom with

$$D_b < v < D_c \tag{5.26}$$

(resp. $-D_c < v < -D_b$), with D_b, D_c given in (5.25), then

$$B < \frac{7M^2 + 2Mm - m^2}{M^2 - m^2} B < V' < C$$

(resp. $-C < V' < -\frac{7M^2 + 2Mm - m^2}{M^2 - m^2} B < -B$).

Proof of Assertion 5.2. Consider $-B < V < B$ and v as given in (5.26). Then, we obtain the following upper and lower bound for the post collision velocity V' from (2.1).

$$\begin{aligned} V' &= \frac{M-m}{M+m}V + \frac{2m}{M+m}v \\ &\stackrel{(5.26)}{<} \frac{M-m}{M+m}B + \frac{2m}{M+m} \left(\frac{M+m}{2m}C - \frac{M-m}{2m}B \right) \\ &= \frac{M-m}{M+m}B + C - \frac{M-m}{M+m}B \\ &= C, \end{aligned}$$

$$\begin{aligned} V' &= \frac{M-m}{M+m}V + \frac{2m}{M+m}v \\ &\stackrel{(5.26)}{>} -\frac{M-m}{M+m}B + \frac{2m}{M+m} \frac{4M^2}{m(M-m)}B \\ &= \frac{-(M-m)^2 + 8M^2}{M^2 - m^2} B \\ &= \frac{7M^2 + 2Mm - m^2}{M^2 - m^2} B \\ &> B \end{aligned}$$

The second case follows analogously. □

Assertion 5.3. If an atom with

$$D_b < v < D_c \tag{5.27}$$

(resp. $-D_c < v < -D_b$), with D_b, D_c given in (5.25) collides with the molecule with $|V| < B$, then $v' < -B$ (resp. $v' > B$).

Proof of Assertion 5.3. Consider (5.27). We obtain the upper bound for the post collision velocity of the atom from (2.2), namely

$$\begin{aligned}
v' &= -\frac{M-m}{M+m}v + \frac{2M}{M+m}V \\
&\stackrel{(5.27)}{<} -\frac{M-m}{M+m} \frac{4M^2}{m(M-m)}B + \frac{2M}{M+m}B \\
&= \frac{-4M^2 + 2Mm}{m(M+m)}B \\
&\leq \frac{-4M^2 + 2M^2}{2m^2}B \\
&< -B.
\end{aligned}$$

The second case follows analogously. □

Assertion 5.4. If an atom enters Λ from the left with

$$D_b < v < D_c \tag{5.28}$$

resp. from the right with

$$-D_c < v < -D_b$$

with D_b, D_c given in (5.25), and the molecule has pre collision velocity $|V| < B$, then the atom stays in Λ no longer than $2t_B$ with t_B given in (5.13).

Proof of Assertion 5.4. Consider the atom entering Λ from the left with (5.28). Note that the proof for atoms entering from the right is analogous.

Since

$$D_b = \frac{4M^2}{m(M-m)}B \geq \frac{4M^2}{M^2}B > B,$$

the atom has velocity $v > B$ until the collision, i.e. the time it takes from entering to the collision is less than t_B . From Assertion 5.3 we obtain for the post collision velocity of the atom that $v' < -B$, i.e. the atom is in the interval no longer than t_B after this collision.

So all in all the atom stays in Λ no longer than $2t_B$.

□

Assertion 5.5. If an atom on the right side (resp. on the left side) of the molecule collides with

$$|v| < \frac{3M - m}{M + m}B \quad (5.29)$$

with the molecule with

$$V > \frac{7M^2 + 2Mm - m^2}{M^2 - m^2}B \quad (5.30)$$

(resp. $V < -\frac{7M^2 + 2Mm - m^2}{M^2 - m^2}B$), then

$$v' > B \text{ (resp. } v' < -B \text{)}.$$

Proof of Assertion 5.5. Consider an atom with (5.29) to the right side of the molecule with (5.30). We obtain the lower bound on the post collision velocity of the atom from (2.2), namely

$$\begin{aligned} v' &= -\frac{M - m}{M + m}v + \frac{2M}{M + m}V \\ &\stackrel{(5.29), (5.30)}{>} -\frac{M - m}{M + m}\frac{3M - m}{M + m}B + \frac{2M}{M + m}\frac{7M^2 + 2Mm - m^2}{M^2 - m^2}B \\ &= \frac{11M^2 + 11M^2m - 7Mm^2 + m^3}{(M^2 - m^2)(M + m)}B \\ &= \frac{10M^2 + 10M^2m - 6Mm^2 + 2m^3 + (M^2 - m^2)(M + m)}{(M^2 - m^2)(M + m)}B \\ &> \frac{4M^2 + 10M^2m + 2m^3 + (M^2 - m^2)(M + m)}{(M^2 - m^2)(M + m)}B \\ &> B. \end{aligned}$$

The second case follows analogously.

□

Assertion 5.6. If an atom on the left side of the molecule collides with

$$v < -B \tag{5.31}$$

with the molecule with

$$V < -\frac{7M^2 + 2Mm - m^2}{M^2 - m^2}B, \tag{5.32}$$

then

$$V' < -\frac{7M^2 + 4Mm + m^2}{(M + m)^2}B < -B \tag{5.33}$$

and

$$v' < -B.$$

Proof of Assertion 5.6. Consider an atom with (5.31) and the molecule with (5.32). By (2.1) it follows that

$$\begin{aligned} V' &= \frac{M - m}{M + m}V + \frac{2m}{M + m}v \\ &< -\frac{M - m}{M + m} \frac{7M^2 + 2Mm - m^2}{M^2 - m^2}B - \frac{2m}{M + m}B \\ &= \frac{-7M^2 - 4Mm - m^2}{(M + m)^2} \\ &= \frac{-5M^2 - 2Mm - (M + m)^2}{(M + m)^2}B \\ &< -B. \end{aligned}$$

Since both, the molecule and the atom, move to the left and the molecule is to the right of the atom, by future collisions the molecule can only (absolutely) speed up the atom, i.e. $v' < -B$. \square

Assertion 5.7. If an atom on the left side of the molecule collides with

$$v < -B \tag{5.34}$$

with the molecule with

$$V' < -\frac{7M^2 + 4Mm + m^2}{(M + m)^2}B \quad (5.35)$$

then

$$V' < \frac{-7M^3 + M^2m - Mm^2 - m^3}{(M + m)^3}B < -B \quad (5.36)$$

and

$$v' < -B.$$

Proof of Assertion 5.7. Consider the atom with (5.34) and the molecule with (5.35). Then, with (2.1) we obtain that

$$\begin{aligned} V' &= \frac{M - m}{M + m}V + \frac{2m}{M + m}v \\ &< -\frac{M - m}{M + m} \frac{7M^2 + 4Mm + m^2}{(M + m)^2}B - \frac{2m}{M + m}B \\ &= \frac{-7M^3 + M^2m - Mm^2 - m^3}{(M + m)^3} \\ &= \frac{-6M^3 + 4M^2m + 2Mm^2 - (M + m)^3}{(M + m)^3}B \\ &< -B. \end{aligned}$$

Since both, the molecule and the atom, move to the left and the molecule is to the right of the atom, the molecule can only (absolutely) speed up the atom, i.e. $v' < -B$. □

Assertion 5.8. If an atom on the left side of the molecule collides with

$$|v| < \frac{3M - m}{M + m}B \quad (5.37)$$

with the molecule with

$$V' < -\frac{7M^2 + 4Mm + m^2}{(M + m)^2}B \quad (5.38)$$

then

$$v' < -B.$$

Proof of Assertion 5.8. Consider an atom on the left side with (5.37) and the molecule with (5.38). Then, by (2.2) we have that

$$\begin{aligned} v' &= -\frac{M-m}{M+m}v + \frac{2M}{M+m}V \\ &< \frac{M-m}{M+m} \frac{3M-m}{M+m} B - \frac{2M}{M+m} \frac{7M^2+4Mm+m^2}{(M+m)^2} B \\ &= \frac{-11M^3 - 9M^2m - 5Mm^2 + m^3}{(M+m)^3} B \\ &< \frac{-8M^3 - 6M^2m - 2Mm^2 - (M+m)^3}{(M+m)^3} B \\ &< -B. \end{aligned}$$

□

Assertion 5.9. If an atom on the left side of the molecule collides with

$$|v| < \frac{3M-m}{M+m} B \tag{5.39}$$

with the molecule with

$$V' < \frac{-7M^3 + M^2m - Mm^2 - m^3}{(M+m)^3} B \tag{5.40}$$

then

$$v' < -B.$$

Proof of Assertion 5.9. Consider an atom with (5.39) and the molecule with (5.40). Then, by (2.2) it follows that

$$v' = -\frac{M-m}{M+m}v + \frac{2M}{M+m}V$$

$$\begin{aligned}
&< \frac{M-m}{M+m} \frac{3M-m}{M+m} B + \frac{2M}{M+m} \frac{-7M^3 + M^2m - Mm^2 - m^3}{(M+m)^3} B \\
&= \frac{-11M^4 + 4M^3m - 6M^2m^2 - 4Mm^3 + m^4}{(M+m)^4} B \\
&= \frac{-10M^4 + 8M^3m + 2m^4 - (M+m)^4}{(M+m)^4} B \\
&< -B.
\end{aligned}$$

□

With these assertions we can show the following.

Lemma 5.4. Let

$$t(\bar{N}) := (\bar{N} + 1) \left(\left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) + 3t_B \quad (5.41)$$

with D_b, D_c given in (5.25) and t_B given in (5.13), then for any $y \in G_{B; \bar{N}; \tilde{v}}$ (cf. (5.16))

$$\Pi_y^{t(\bar{N})}(G_{B,C;0}) \geq C_2 e^{-C_3 \bar{N}} \quad (5.42)$$

with

$$C_2 := \exp \left(-2\rho \left(\left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + 4t_B \right) (\sqrt{2\pi\mathcal{K}m})^{-1} \right) \quad (5.43)$$

$$C_3 := 2\rho \left(\left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) (\sqrt{2\pi\mathcal{K}m})^{-1}. \quad (5.44)$$

Proof of Lemma 5.4. Recall that $G_{B; \bar{N}; \tilde{v}}$ are the configurations where $|V| < B$, the number of atoms in Λ is less or equal \bar{N} and the speed of the atoms is less than $\tilde{v} = \frac{3M-m}{M+m} B$. For ease of notation we set $t = 0$ for the time of the following situation. Note that throughout this section, whenever we set $t = 0$, it is the time of a situation and not the beginning of the process. Consider $Y(0) = y \in G_{B; \bar{N}; \tilde{v}}$. Denote by N_r^y and N_l^y the number of atoms to

the right resp. to the left of the molecule at time $t = 0$. Note that

$$N_r^y + N_l^y \leq \bar{N}.$$

First, we let atoms enter Λ from the left to let the molecule push out the atoms, which are to the right of it. The entering atoms have velocity

$$D_b < v < D_c, \tag{5.45}$$

with D_b, D_c given in (5.25), and shall enter Λ according to the following prescription. Note that no other atom shall enter the interval during this procedure.

Let $\bar{\Delta} > 0$. The first atom enters Λ during $[0, \bar{\Delta}]$ and no atom enters during $[\bar{\Delta}, \bar{\Delta} + t_B]$. By time $\bar{\Delta} + t_B$ the molecule has either reached L (and has velocity $|V| < C$ (cf. Assertion 5.2)) or if not, it was slowed down to a speed less than B by some atoms of the right side. At least one of the N_r^y atoms will have left Λ by time $\bar{\Delta} + t_B$: In the first case it is trivial, since then all atoms from the right have left Λ . In the latter case at least the atom, which collided at first with the molecule on the r.h.s. will be kicked out, since this atom has pre collision velocity $|v| < \frac{3M-m}{M+m}B$ (by definition of $G_{B;\bar{N};\bar{v}}$) and the molecule collides with $V > \frac{7M^2+2Mm-m^2}{M^2-m^2}B$ (see Assertion 5.2), such that by Assertion 5.5 it follows that $v' > B$. Note that the atom which we have send in may enter the interval latest at time $\bar{\Delta}$ and has velocity $v > D_b > B$. This atom then collides with the molecule, which gain post collision velocity $V > B$. Since the molecule causes a post collision velocity $v' > B$ of the atom to its right, it doesn't take longer than t_B from the entering of the atom, which we have send in to the leaving time of the atom to the right of the molecule. Hence, by time $\bar{\Delta} + t_B$ at least one atom of the r.h.s. of the molecule has left Λ .

If there are still atoms to the right of the molecule, another atom with (5.45) enters during $[\bar{\Delta} + t_B, 2\bar{\Delta} + t_B]$ and no atom during $[2\bar{\Delta} + t_B, 2(\bar{\Delta} + t_B)]$, etc. until all N_r^y atoms are pushed out, i.e.

$$t_r^y := N_r^y(\bar{\Delta} + t_B) \tag{5.46}$$

is an upper bound on the time it takes with this procedure to reach a state where no atom is to the right of the molecule and $|V| < C$. The latter follows by Assertion 5.2. Note that as soon as by a time $m(\bar{\Delta} + t_B)$, $m \in \{1, \dots, N_r^y - 1\}$ there are no atoms to the right of the molecule, we consider the event, that no atom enters during $[m(\bar{\Delta} + t_B), t_r^y]$.

If $|V(t_r^y)| < B$, we send in one additional atom from the left during $[t_r^y, t_r^y + \bar{\Delta}]$ with (5.45) (so that $B < V' < C$ (cf. Assertion 5.2)), and no atom during $[t_r^y + \bar{\Delta}, t_r^y + \bar{\Delta} + 2t_B]$. If $B < |V(t_r^y)| < C$, no atom enters during $[t_r^y, t_r^y + \bar{\Delta} + 2t_B]$. Then, in both cases by time

$$t_r^y + \bar{\Delta} + 2t_B = (N_r^y + 1)(\bar{\Delta} + t_B) + t_B \tag{5.47}$$

the molecule was reflected at L , latest at time

$$t_r^y + \bar{\Delta} + t_B, \tag{5.48}$$

and has either reached $-L$ (and has velocity $|V| < C$), or if not, it was slowed down to a speed less than B by some of the atoms on the left. Note that at time (5.48) there are $N_l^y + 2$ atoms or less on the l.h.s. of the molecule in Λ , since an atom which is send in during $[(N_r^y - 1)(\bar{\Delta} + t_B), (N_r^y - 1)(\bar{\Delta} + t_B) + \bar{\Delta}]$ or $[t_r^y, t_r^y + \bar{\Delta}]$ may be still in the interval (with $v < -B$ (cf. Assertion 5.3)). But in any case these two atoms and at least one of the N_l^y atoms on the left have left Λ by time (5.47). This follows by similar arguments as before: If the molecule has reached $-L$, all atoms on the left were pushed out. If the molecule didn't reach $-L$, it must have been slowed down to a speed less than B by at least one atom of the l.h.s.. In the latter case there are three possible situations which may occur: After the reflection of the molecule at L (i) the first two collisions of the molecule are with the two atoms which were send in during the procedure. Note that the pre collision velocity of both atoms is $v < -B$; (ii) the molecule first collides with one of the atoms which were send in during the procedure and second with one of the N_l^y atoms; (iii) the first collision of the molecule is with one of the N_l^y atoms.

To prove that at least the three atoms will have left Λ by time (5.47), it is enough to show that $V < -B$ from the time of reflection at L (latest at time (5.48)) until the time where all three atoms have $v < -B$, since then it takes no longer than t_B from the reflection until all three atoms will have left the interval, i.e. all three atoms will have left the interval by time (5.47). We show that now.

By Assertion 5.6 and Assertion 5.7 it follows that in (i) the post collision velocity of the atoms of the first and second collision is $v' < -B$. Furthermore the upper bound of the post collision velocity of the molecule after the first two collisions is given by (5.36) and in particular $V < -B$ from the time of reflection at L on. By Assertion 5.9 it follows that the post collision velocity of the atom of the third collision is $v' < -B$. i.e. all three atoms with which the molecule collided with have $v' < -B$. Hence, all three atoms leave the interval by time (5.47). In (ii) the atom of the first collision has $v' < -B$ and the upper bound of the post collision velocity of the molecule is given in (5.33) in particular $V < -B$ (cf. Assertion 5.6). By Assertion 5.8 the atom of the second collision has also $v' < -B$. Since the second atom we have send in during the procedure has already $v < -B$ after the first collision with the molecule and will keep $v < -B$ no matter if it collides with the molecule again or not, all in all we have that $V < -B$ until all three atoms have $v < -B$, i.e. these atoms will have left the interval before (5.47). In (iii) the atom of the first collision obtains by the collision with the molecule $v' < -B$ (cf. Assertion 5.5). Since both atoms which were send in during the procedure have already $v < -B$ (by the first collision), all three atoms leave the interval before (5.47). This gives the conjecture, namely by time (5.47) at least one of the N_l^y atoms and both atoms which were send in during the procedure have left the interval by (5.47).

We now continue in a similar way as before: If by time (5.47) there are still atoms to the left (not more than $N_l^y - 1$), we push out the remaining atoms, but now by atoms entering Λ from the right with $-D_c < v < -D_b$. Hence, by time

$$(N_r^y + 1)(\bar{\Delta} + t_B) + t_B + (N_l^y - 1)(\bar{\Delta} + t_B) + t_B$$

$$= (N_r^y + N_l^y)(\bar{\Delta} + t_B) + 2t_B \quad (5.49)$$

the molecule is alone in Λ with $|V| < C$, since then also the last incoming atom has left Λ again.

If $|V(t)| < B$ with t given in (5.49) we send in one additional atom from the left with $D_b < v < D_c$ during

$$[(N_r^y + N_l^y)(\bar{\Delta} + t_B) + 2t_B, (N_r^y + N_l^y + 1)(\bar{\Delta} + t_B) + t_B]$$

and no atom during

$$[(N_r^y + N_l^y + 1)(\bar{\Delta} + t_B) + t_B, (N_r^y + N_l^y + 1)(\bar{\Delta} + t_B) + 3t_B].$$

If $B < |V(t)| < C$ for t given in (5.49) we consider the event that no atoms enter during $[(N_r^y + N_l^y)(\bar{\Delta} + t_B) + 2t_B, (N_r^y + N_l^y + 1)(\bar{\Delta} + t_B) + 3t_B]$.

It follows by Assertion 5.2 that by time

$$(N_r^y + N_l^y + 1)(\bar{\Delta} + t_B) + 3t_B \quad (5.50)$$

the molecule is alone in Λ with velocity $B < |V| < C$.

Since $N_r^y + N_l^y \leq \bar{N}$ for any $y \in G_{B;\bar{N};\bar{v}}$, it follows from (5.50) that

$$\bar{\Delta}_{\bar{N}} := (\bar{N} + 1)(\bar{\Delta} + t_B) + 3t_B, \quad (5.51)$$

is an upper bound on the time it takes with the above procedure to reach a state where the molecule is alone in Λ with velocity $B < |V| < C$ for any $y \in G_{B;\bar{N};\bar{v}}$.

By the above procedure we can estimate $\Pi_y^{\bar{\Delta}_{\bar{N}}}(G_{B,C;0})$ for $y \in G_{B;\bar{N};\bar{v}}$ with $\bar{\Delta}_{\bar{N}}$ given in (5.51), and we obtain Lemma 5.4: Since \mathcal{M}_t is a stationary Markov process

$$\Pi_y^{\bar{\Delta}_{\bar{N}}}(G_{B,C;0}) \quad (5.52)$$

$$\begin{aligned} &\stackrel{(5.51)}{=} \Pi_y^{(\bar{N}+1)(\bar{\Delta}+t_B)+3t_B}(G_{B,C;0}) \\ &= \Pi_y^{(N_r^y+N_l^y+1)(\bar{\Delta}+t_B)+3t_B+(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}+t_B)}(G_{B,C;0}) \\ &= \int \Pi_y^{(N_r^y+N_l^y+1)(\bar{\Delta}+t_B)+3t_B}(dy') \Pi_{y'}^{(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}+t_B)}(G_{B,C;0}) \\ &\geq \int_{G_{B,C;0}} \Pi_y^{(N_r^y+N_l^y+1)(\bar{\Delta}+t_B)+3t_B}(dy') \Pi_{y'}^{(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}+t_B)}(G_{B,C;0}). \end{aligned} \quad (5.53)$$

Any $Y(0) = y \in G_{B,C;0}$ will stay in $G_{B,C;0}$ until time $(\bar{N} - (N_r^y + N_l^y))(\bar{\Delta} + t_B)$ if no atom enters Λ during $[0, (\bar{N} - (N_r^y + N_l^y))(\bar{\Delta} + t_B)]$, so that we can estimate

$$\begin{aligned} (5.53) &\geq \int_{G_{B,C;0}} \Pi_y^{(N_r^y+N_l^y+1)(\bar{\Delta}+t_B)+3t_B}(dy') \\ &\quad \cdot \mu(\{\mathcal{N}(\bar{N} - (N_r^y + N_l^y))(\bar{\Delta} + t_B) = 0\}) \end{aligned}$$

$$\begin{aligned}
&= \Pi_y^{(N_r^y + N_l^y + 1)(\bar{\Delta} + t_B) + 3t_B}(G_{B,C;0}) \cdot \\
&\quad \cdot \mu(\{\mathcal{N}(\bar{N} - (N_r^y + N_l^y))(\bar{\Delta} + t_B) = 0\})
\end{aligned} \tag{5.54}$$

To estimate further we start with

$$\begin{aligned}
&\Pi_y^{(N_r^y + N_l^y + 1)(\bar{\Delta} + t_B) + 3t_B}(G_{B,C;0}) = \\
&= \int \Pi_y^{(N_r^y + N_l^y)(\bar{\Delta} + t_B) + 2t_B}(dy') \Pi_{y'}^{\bar{\Delta} + 2t_B}(G_{B,C;0}) \\
&\geq \int_{G_{B;0} \cup G_{B,C;0}} \Pi_y^{(N_r^y + N_l^y)(\bar{\Delta} + t_B) + 2t_B}(dy') \Pi_{y'}^{\bar{\Delta} + 2t_B}(G_{B,C;0}),
\end{aligned} \tag{5.55}$$

where $G_{B;0} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ is the set of configurations where the molecule is alone with $|V| < B$, i.e. with ease of notation

$$G_{B;0} = \{|V| < B, N = 0\}.$$

Since for $y' \in G_{B;0}$ resp. $y' \in G_{B,C;0}$ different procedures are necessary to reach by time $\bar{\Delta} + 2t_B$ a state in $G_{B,C;0}$, we treat these cases separately when estimating the second factor of (5.55). Note since Lemma 5.4 requires a uniform lower bound for the transitions, we need the same estimate in both cases. We will get that by making an explicit choice for $\bar{\Delta}$ later on. We can make this choice, since until now the only condition on $\bar{\Delta}$ is its positivity. If $Y(0) = y' \in G_{B,C;0}$ and no atom enters during $[0, \bar{\Delta} + 2t_B]$, then $Y(\bar{\Delta} + 2t_B) \in G_{B,C;0}$. So it follows for $y' \in G_{B,C;0}$ that

$$\Pi_{y'}^{\bar{\Delta} + 2t_B}(G_{B,C;0}) \geq \mu(\{\mathcal{N}(\bar{\Delta} + 2t_B) = 0\}). \tag{5.56}$$

Now we show that also transitions starting at $Y(0) = y' \in G_{B;0}$ can be estimated by the same bound as given in (5.56). We know from the above, sending in one atom from the left with $D_b < v < D_c$ during $[0, \bar{\Delta}]$ and no atom during $[\bar{\Delta}, \bar{\Delta} + 2t_B]$ yields to $Y(\bar{\Delta} + 2t_B) \in G_{B,C;0}$. So denote by $Q \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ the set of configurations which are possible for the system at time $\bar{\Delta}$ if it starts at $t = 0$ in $G_{B;0}$ and one atom from the left enters with $D_b < v < D_c$ during $[0, \bar{\Delta}]$, i.e. with ease of notation

$$Q = \{\text{There is no or one atom in } \Lambda.$$

If there is one atom, it is on the l.h.s. of the molecule

with velocity $D_b < v < D_c$ or $v < -B$.

If $D_b < v < D_c$, then $|V| < B$;

if $v < -B$, then $B < |V| < C$.

If there's no atom in Λ , $B < |V| < C$).

Since any $Y(0) = y'' \in Q$ reaches a state in $G_{B,C;0}$ at time $2t_B$ if no atom enters during

$[0, 2t_B]$ we have that

$$\Pi_{y'}^{\bar{\Delta}+2t_B}(G_{B,C;0}) = \int \Pi_{y'}^{\bar{\Delta}}(dy'') \Pi_{y''}^{2t_B}(G_{B,C;0}) \quad (5.57)$$

$$\begin{aligned} &\geq \int_Q \Pi_{y'}^{\bar{\Delta}}(dy'') \Pi_{y''}^{2t_B}(G_{B,C;0}) \\ &\geq \int_Q \Pi_{y'}^{\bar{\Delta}}(dy'') \mu(\{\mathcal{N}(2t_B) = 0\}) \\ &= \Pi_{y'}^{\bar{\Delta}}(Q) \mu(\{\mathcal{N}(2t_B) = 0\}). \end{aligned} \quad (5.58)$$

To estimate the first factor in (5.58) we note that for $y' \in G_{B;0}$

$$\Pi_{y'}^{\bar{\Delta}}(Q) \geq \mu(\{\mathcal{N}_{D_b, D_c}(\bar{\Delta}) = 1\}) \mu(\{\mathcal{N}_{D_c, \infty}(\bar{\Delta}) = 0\}) \mu(\{\mathcal{N}_{-\infty, D_b}(\bar{\Delta}) = 0\}), \quad (5.59)$$

since $Y(0) = y' \in G_{B;0}$ is in Q by time $\bar{\Delta}$ if exactly one atom enters during $[0, \bar{\Delta}]$ and has $D_b < v < D_c$. Having in mind that (5.57) shall be estimated such that it has the same lower bound as (5.56), we make an explicit choice for $\bar{\Delta}$. Note that (5.56) is valid for any $\bar{\Delta} > 0$. Let

$$\bar{\Delta}_{bc} := \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1}, \quad (5.60)$$

where ρ is the density of the ideal gas and $f(v)$ is the Maxwellian (cf. (2.5)). Then, the expected number of atoms entering Λ during a time interval of length $\bar{\Delta}_{bc}$ with velocity $D_b < v < D_c$ is

$$\mathbb{E}(\mathcal{N}_{D_b, D_c}(\bar{\Delta}_{bc})) = \bar{\Delta}_{bc} \rho \int_{D_b}^{D_c} v f(v) dv \stackrel{(5.60)}{=} 1.$$

If we choose

$$\bar{\Delta} = \bar{\Delta}_{bc}, \quad (5.61)$$

for estimating (5.59) we can use the monotonicity of Poisson random variables: If the random variable X is Poisson-distributed with mean λ , then for any $j, k \in \mathbb{N}$ with $j \leq k \leq \lambda$

$$\mathbb{P}(X = j) \leq \mathbb{P}(X = k) \leq \mathbb{P}(X = \lambda). \quad (5.62)$$

With (5.61) it follows that

$$(5.59) \geq \mu(\{\mathcal{N}_{D_b, D_c}(\bar{\Delta}_{bc}) = 0\}) \mu(\{\mathcal{N}_{D_c, \infty}(\bar{\Delta}_{bc}) = 0\}) \mu(\{\mathcal{N}_{-\infty, D_b}(\bar{\Delta}_{bc}) = 0\}). \quad (5.63)$$

Since $\mathcal{N}_{D_b, D_c}(\bar{\Delta}_{bc})$, $\mathcal{N}_{D_c, \infty}(\bar{\Delta}_{bc})$ and $\mathcal{N}_{-\infty, D_b}(\bar{\Delta}_{bc})$ are independent (cf. (2.7))

$$\Pi_{y'}^{\bar{\Delta}_{bc}}(Q) \geq \mu(\{\mathcal{N}(\bar{\Delta}_{bc}) = 0\}). \quad (5.64)$$

By (5.58) and (5.64) we get for the second factor of (5.55) for $y' \in G_{B;0}$

$$\Pi_{y'}^{\bar{\Delta}_{bc}+2t_B}(G_{B,C;0}) \geq \mu(\{\mathcal{N}(\bar{\Delta}_{bc}) = 0\})\mu(\{\mathcal{N}(t_B) = 0\}). \quad (5.65)$$

To continue estimating the r.h.s. of (5.65), note following fact. Denote by $|[a, b]|$ the length of the time interval $[a, b]$, then

$$\mu(\{\mathcal{N}([a, b])\}) = \mu(\{\mathcal{N}([t, t + |[a, b]|])\}). \quad (5.66)$$

Using (5.66), we obtain for the r.h.s. of (5.65) that

$$\begin{aligned} & \mu(\{\mathcal{N}(\bar{\Delta}_{bc}) = 0\})\mu(\{\mathcal{N}(t_B) = 0\}) \\ & \stackrel{(5.66)}{=} \mu(\{\mathcal{N}([0, \bar{\Delta}_{bc}]) = 0\})\mu(\{\mathcal{N}([\bar{\Delta}_{bc}, \bar{\Delta}_{bc} + t_B]) = 0\}) \\ & \stackrel{(2.7)}{=} \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + t_B) = 0\}), \end{aligned} \quad (5.67)$$

and altogether for (5.65) with $y' \in G_{B;0}$ by (5.67) that

$$\Pi_{y'}^{\bar{\Delta}_{bc}+2t_B}(G_{B,C;0}) \geq \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + t_B) = 0\}).$$

Choosing (5.61), we obtain also for (5.56) with $y' \in G_{B,C;0}$ the same estimate, namely

$$\Pi_{y'}^{\bar{\Delta}_{bc}+2t_B}(G_{B,C;0}) \geq \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 2t_B) = 0\}).$$

Plugging this into (5.55), we get

$$\begin{aligned} (5.55) & \geq \int_{G_{B;0} \cup G_{B,C;0}} \Pi_y^{(N_r^y + N_l^y)(\bar{\Delta}_{bc} + t_B) + 2t_B}(dy') \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 2t_B) = 0\}) \\ & = \Pi_y^{(N_r^y + N_l^y)(\bar{\Delta}_{bc} + t_B) + 2t_B}(G_{B;0} \cup G_{B,C;0}) \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 2t_B) = 0\}). \end{aligned} \quad (5.68)$$

We continue with

$$\begin{aligned} & \Pi_y^{(N_r^y + N_l^y)(\bar{\Delta}_{bc} + t_B) + 2t_B}(G_{B;0} \cup G_{B,C;0}) \\ & = \Pi_y^{(N_r^y + 1)(\bar{\Delta}_{bc} + t_B) + t_B + (N_l^y - 1)(\bar{\Delta}_{bc} + t_B) + t_B}(G_{B;0} \cup G_{B,C;0}) \\ & = \int \Pi_y^{(N_r^y + 1)(\bar{\Delta}_{bc} + t_B) + t_B + (N_l^y - 1)(\bar{\Delta}_{bc} + t_B)}(dy') \Pi_{y'}^{t_B}(G_{B;0} \cup G_{B,C;0}). \end{aligned} \quad (5.69)$$

Denote by $R \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ the set of configurations which are possible for the system at time

$$(N_r^y + 1)(\bar{\Delta}_{bc} + t_B) + t_B + (N_l^y - 1)(\bar{\Delta}_{bc} + t_B),$$

starting at $t = 0$ in $G_{B;\bar{N};\bar{v}}$ and undergoing the procedure which was described underneath

(5.45), i.e. we have that

$$R = \left\{ \begin{array}{l} \text{There is no or one atom in the interval.} \\ \text{If there is one atom, it is to the right of the molecule} \\ \text{and has velocity } v > B. \\ \text{The molecule has velocity } |V| < C. \end{array} \right\}.$$

Hence,

$$(5.69) \geq \int_R \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc+t_B})+t_B+(N_l^y-1)(\bar{\Delta}_{bc+t_B})}(dy') \Pi_{y'}^{t_B}(G_{B;0} \cup G_{B,C;0}). \quad (5.70)$$

Since for $Y(0) = y' \in R$, if no atom enters during $[0, t_B]$ then $Y(t_B) \in G_{B;0} \cup G_{B,C;0}$, i.e.

$$\begin{aligned} (5.70) &\geq \int_R \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc+t_B})+t_B+(N_l^y-1)(\bar{\Delta}_{bc+t_B})}(dy') \mu(\{\mathcal{N}(t_B) = 0\}) \\ &= \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc+t_B})+t_B+(N_l^y-1)(\bar{\Delta}_{bc+t_B})}(R) \mu(\{\mathcal{N}(t_B) = 0\}). \end{aligned} \quad (5.71)$$

Now we start with

$$\Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc+t_B})+t_B+(N_l^y-1)(\bar{\Delta}_{bc+t_B})}(R) \quad (5.72)$$

$$\begin{aligned} &= \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc+t_B})+t_B+(N_l^y-2)(\bar{\Delta}_{bc+t_B})+(\bar{\Delta}_{bc+t_B})}(R) \\ &= \int \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc+t_B})+t_B+(N_l^y-2)(\bar{\Delta}_{bc+t_B})}(dy') \Pi_{y'}^{\bar{\Delta}_{bc+t_B}}(R). \end{aligned} \quad (5.73)$$

Starting at $t = 0$ in $G_{B;\bar{N};\tilde{v}}$ and undergoing the procedure as described underneath (5.45), at time $(N_r^y + 1)(\bar{\Delta}_{bc} + t_B) + t_B + (N_l^y - 2)(\bar{\Delta}_{bc} + t_B)$ either the molecule is alone with $|V| < C$, or there is one atom to the the left (with $|v| < \tilde{v}$) and $|V| < B$. To estimate (5.73) we denote by $G_{C,0} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ the set of configurations where the molecule is alone in the interval with $|V| < C$, i.e. with ease of notation

$$G_{C,0} := \{|V| < C, N = 0\},$$

and by $G_{B;n,0;\tilde{v}} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ the set of configurations where $|V| < B$, no more than n atoms are to the left of the molecule, each with $|v| < \tilde{v}$, and no atom to the right, i.e. with ease of notation

$$G_{B;n,0;\tilde{v}} := \{|V| < B; N_l \leq n; N_r = 0; |v| < \tilde{v}\}.$$

Then, we have for (5.73) that

$$\int \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc+t_B})+t_B+(N_l^y-2)(\bar{\Delta}_{bc+t_B})}(dy') \Pi_{y'}^{\bar{\Delta}_{bc+t_B}}(R)$$

$$\geq \int_{G_{C,0} \cup G_{B;1,0;\bar{v}}} \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-2)(\bar{\Delta}_{bc}+t_B)}(dy') \Pi_{y'}^{\bar{\Delta}_{bc}+t_B}(R). \quad (5.74)$$

If no atom enters Λ during $[0, \bar{\Delta}_{bc} + t_B]$, $Y(0) = y' \in G_{C,0}$ stays in $G_{C,0}$ until time $\bar{\Delta}_{bc} + t_B$. Since $G_{C,0} \subset R$, we have

$$\Pi_{y'}^{\bar{\Delta}_{bc}+t_B}(R) \geq \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + t_B) = 0\}) \quad (5.75)$$

for $y' \in G_{C,0}$.

Since $Y(0) = y' \in G_{B;1,0;\bar{v}}$ reaches by time $\bar{\Delta}_{bc} + t_B$ a state in R if exactly one atom with $-D_c < v < -D_b$ enters during $[0, \bar{\Delta}_{bc}]$ and no atom during $[\bar{\Delta}_{bc}, \bar{\Delta}_{bc} + t_B]$, we get by the same arguments which gave (5.63), (5.65) resp. (5.67), for $y' \in G_{B;1,0;\bar{v}}$

$$\begin{aligned} & \Pi_{y'}^{\bar{\Delta}_{bc}+t_B}(R) \\ & \geq \mu(\{\mathcal{N}_{-D_c, -D_b}(\bar{\Delta}_{bc}) = 1\}) \mu(\{\mathcal{N}_{-\infty, -D_c}(\bar{\Delta}_{bc}) = 0\}) \cdot \\ & \quad \cdot \mu(\{\mathcal{N}_{-D_b, \infty}(\bar{\Delta}_{bc}) = 0\}) \mu(\{\mathcal{N}(t_B) = 0\}) \\ & \stackrel{(5.62)}{\geq} \mu(\{\mathcal{N}_{-D_c, -D_b}(\bar{\Delta}_{bc}) = 0\}) \mu(\{\mathcal{N}_{-\infty, -D_c}(\bar{\Delta}_{bc}) = 0\}) \cdot \\ & \quad \cdot \mu(\{\mathcal{N}_{-D_b, \infty}(\bar{\Delta}_{bc}) = 0\}) \mu(\{\mathcal{N}(t_B) = 0\}) \\ & \geq \mu(\{\mathcal{N}(\bar{\Delta}_{bc}) = 0\}) \mu(\{\mathcal{N}(t_B) = 0\}) \\ & \stackrel{(5.66), (2.7)}{=} \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + t_B) = 0\}). \end{aligned} \quad (5.76)$$

We then have with (5.75) and (5.76) for $y' \in G_{C,0} \cup G_{B;1,0;\bar{v}}$ that

$$\Pi_{y'}^{\bar{\Delta}_{bc}+t_B}(R) \geq \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + t_B) = 0\}), \quad (5.77)$$

which we use to continue estimating (5.74):

$$\begin{aligned} (5.74) &= \int_{G_{C,0} \cup G_{B;1,0;\bar{v}}} \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-2)(\bar{\Delta}_{bc}+t_B)}(dy') \Pi_{y'}^{\bar{\Delta}_{bc}+t_B}(R) \\ & \stackrel{(5.77)}{\geq} \int_{G_{C,0} \cup G_{B;1,0;\bar{v}}} \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-2)(\bar{\Delta}_{bc}+t_B)}(dy') \cdot \\ & \quad \cdot \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + t_B) = 0\}) \\ &= \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-2)(\bar{\Delta}_{bc}+t_B)}(G_{C,0} \cup G_{B;1,0;\bar{v}}) \cdot \\ & \quad \cdot \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + t_B) = 0\}). \end{aligned} \quad (5.78)$$

Estimating

$$\Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-2)(\bar{\Delta}_{bc}+t_B)}(G_{C,0} \cup G_{B;1,0;\bar{v}}) \quad (5.79)$$

in a similar way as (5.72), we obtain that

$$\begin{aligned}
& \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-2)(\bar{\Delta}_{bc}+t_B)}(G_{C,0} \cup G_{B;1,0;\bar{v}}) \\
&= \int \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-3)(\bar{\Delta}_{bc}+t_B)}(dy') \Pi_{y'}^{\bar{\Delta}_{bc}+t_B}(G_{C,0} \cup G_{B;1,0;\bar{v}}) \\
&\geq \int_{G_{C,0} \cup G_{B;2,0;\bar{v}}} \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-3)(\bar{\Delta}_{bc}+t_B)}(dy') \\
&\quad \cdot \Pi_{y'}^{\bar{\Delta}_{bc}+t_B}(G_{C,0} \cup G_{B;1,0;\bar{v}}) \\
&\geq \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-3)(\bar{\Delta}_{bc}+t_B)}(G_{C,0} \cup G_{B;2,0;\bar{v}}) \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + t_B) = 0\}).
\end{aligned}$$

Repeating the splitting on

$$\Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-3)(\bar{\Delta}_{bc}+t_B)}(G_{C,0} \cup G_{B;2,0;\bar{v}}),$$

we finally obtain for (5.79) by (2.7) and using (5.66) that

$$\begin{aligned}
& \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-2)(\bar{\Delta}_{bc}+t_B)}(G_{C,0} \cup G_{B;1,0;\bar{v}}) \\
&\geq \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B}(G_{C,0} \cup G_{B;N_l^y-1,\bar{v}}) \mu(\{\mathcal{N}((N_l^y - 2)(\bar{\Delta}_{bc} + t_B)) = 0\}). \quad (5.80)
\end{aligned}$$

Now we estimate

$$\begin{aligned}
& \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B}(G_{C,0} \cup G_{B;N_l^y-1,0;\bar{v}}) \\
&= \int \Pi_y^{N_r^y}(\bar{\Delta}_{bc}+t_B)(dy') \Pi_{y'}^{\bar{\Delta}_{bc}+2t_B}(G_{C,0} \cup G_{B;N_l^y-1,0;\bar{v}}) \\
&\geq \int_{G_{C;N_l^y,0;\bar{v};2,-B}} \Pi_y^{N_r^y}(\bar{\Delta}_{bc}+t_B)(dy') \Pi_{y'}^{\bar{\Delta}_{bc}+2t_B}(G_{C,0} \cup G_{B;N_l^y-1,0;\bar{v}}) \\
&= \int_{G_{B;N_l^y,0;\bar{v};2,-B} \cup G_{B,C;N_l^y,0;\bar{v};2,-B}} \Pi_y^{N_r^y}(\bar{\Delta}_{bc}+t_B)(dy') \Pi_{y'}^{\bar{\Delta}_{bc}+2t_B}(G_{C,0} \cup G_{B;N_l^y-1,0;\bar{v}}), \quad (5.81)
\end{aligned}$$

where $G_{C;N_l^y,0;\bar{v};2,-B} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ denotes the set where $|V| < C$, no more than N_l^y atoms with $|v| < \bar{v}$ and no more than 2 atoms with $v < -B$ are to the left of the molecule. If $Y(0) = y' \in G_{B,C;N_l^y,0;\bar{v};2,-B}$ and no atom enters Λ during $[0, \bar{\Delta}_{bc} + 2t_B]$, then either $Y(\bar{\Delta}_{bc} + 2t_B) \in G_{C,0}$ or $Y(\bar{\Delta}_{bc} + 2t_B) \in G_{B;N_l^y-1,0;\bar{v}}$. This follows by arguments we gave underneath (5.46). We then have that

$$\Pi_{y'}^{\bar{\Delta}_{bc}+2t_B}(G_{C,0} \cup G_{B;N_l^y-1,0;\bar{v}}) \geq \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 2t_B) = 0\}) \quad (5.82)$$

for $y' \in G_{B,C;N_l^y,0;\bar{v};2,-B}$.

If $Y(0) = y' \in G_{B;N_l^y,0;\bar{v};2,-B}$ and exactly one atom with $D_b < v < D_c$ enters during $[0, \bar{\Delta}_{bc}]$ from the left, and no atom during $[\bar{\Delta}_{bc}, \bar{\Delta}_{bc} + 2t_B]$, then either $Y(\bar{\Delta}_{bc} + 2t_B) \in G_{C,0}$ or

$Y(\bar{\Delta}_{bc} + 2t_B) \in G_{B;N_l^y-1,0;\bar{v}}$, so that for $y' \in G_{B;N_l^y,0;\bar{v};2,-B}$

$$\Pi_{y'}^{\bar{\Delta}_{bc}+2t_B}(G_{C,0} \cup G_{B;N_l^y-1,0;\bar{v}}) \geq \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 2t_B) = 0\}). \quad (5.83)$$

Inequalities (5.82) and (5.83) yield that

$$\begin{aligned} (5.81) &= \int_{G_{B;N_l^y,0;\bar{v};2,-B} \cup G_{B,C;N_l^y,0;\bar{v};2,-B}} \Pi_y^{N_r^y(\bar{\Delta}_{bc}+t_B)}(dy') \Pi_{y'}^{\bar{\Delta}_{bc}+2t_B}(G_{C,0} \cup G_{B;N_l^y-1,0;\bar{v}}) \\ &\geq \int_{G_{B;N_l^y,0;\bar{v};2,-B} \cup G_{B,C;N_l^y,0;\bar{v};2,-B}} \Pi_y^{N_r^y(\bar{\Delta}_{bc}+t_B)}(dy') \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 2t_B) = 0\}) \\ &= \Pi_y^{N_r^y(\bar{\Delta}_{bc}+t_B)}(G_{C;N_l^y,0;\bar{v}}) \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 2t_B) = 0\}). \end{aligned} \quad (5.84)$$

By the similar splitting which yielded (5.80), we can estimate

$$\Pi_y^{N_r^y(\bar{\Delta}_{bc}+t_B)}(G_{C;N_l^y,0;\bar{v};2,-B}) \geq \mu(\{\mathcal{N}(N_r^y(\bar{\Delta}_{bc} + t_B)) = 0\}). \quad (5.85)$$

Finally, we obtain for (5.52) for any $y \in G_{B;\bar{N};\bar{v}}$ that

$$\Pi_y^{\bar{\Delta}_{\bar{N}}}(G_{B,C;0}) \quad (5.86)$$

$$\begin{aligned} &\stackrel{(5.51)}{=} \Pi_y^{(\bar{N}+1)(\bar{\Delta}_{bc}+t_B)+3t_B}(G_{B,C;0}) \\ &= \Pi_y^{(N_r^y+N_l^y+1)(\bar{\Delta}_{bc}+t_B)+3t_B+(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}_{bc}+t_B)}(G_{B,C;0}) \\ &\stackrel{(5.54)}{\geq} \Pi_y^{(N_r^y+N_l^y+1)(\bar{\Delta}_{bc}+t_B)+3t_B}(G_{B,C;0}) \cdot \\ &\quad \cdot \mu(\{\mathcal{N}(\bar{N} - (N_r^y + N_l^y))(\bar{\Delta}_{bc} + t_B) = 0\}) \\ &\stackrel{(5.68)}{\geq} \Pi_y^{(N_r^y+N_l^y)(\bar{\Delta}_{bc}+t_B)+2t_B}(G_{B;0} \cup G_{B,C;0}) \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 2t_B) = 0\}) \\ &\quad \cdot \mu(\{\mathcal{N}(\bar{N} - (N_r^y + N_l^y))(\bar{\Delta}_{bc} + t_B) = 0\}) \\ &= \Pi_y^{(N_r^y+N_l^y)(\bar{\Delta}_{bc}+t_B)+2t_B}(G_{B;0} \cup G_{B,C;0}) \cdot \\ &\quad \cdot \mu(\{\mathcal{N}((\bar{\Delta}_{bc} + 2t_B) + (\bar{N} - (N_r^y + N_l^y))(\bar{\Delta}_{bc} + t_B)) = 0\}) \end{aligned} \quad (5.87)$$

$$\begin{aligned} &\stackrel{(5.71)}{\geq} \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-1)(\bar{\Delta}_{bc}+t_B)}(R) \mu(\{\mathcal{N}(t_B) = 0\}) \cdot \\ &\quad \cdot \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 2t_B + (\bar{N} - (N_r^y + N_l^y))(\bar{\Delta}_{bc} + t_B)) = 0\}) \\ &= \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-1)(\bar{\Delta}_{bc}+t_B)}(R) \cdot \\ &\quad \cdot \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 3t_B + (\bar{N} - (N_r^y + N_l^y))(\bar{\Delta}_{bc} + t_B)) = 0\}) \\ &\stackrel{(5.78)}{\geq} \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-2)(\bar{\Delta}_{bc}+t_B)}(G_{C,0} \cup G_{B;1,0;\bar{v}}) \cdot \\ &\quad \cdot \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + t_B) = 0\}) \cdot \\ &\quad \cdot \mu(\{\mathcal{N}(\bar{\Delta}_{bc} + 3t_B + (\bar{N} - (N_r^y + N_l^y))(\bar{\Delta}_{bc} + t_B)) = 0\}) \end{aligned} \quad (5.88)$$

$$\begin{aligned}
&= \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B+(N_l^y-2)(\bar{\Delta}_{bc}+t_B)}(G_{C,0} \cup G_{B;1,0;\bar{v}}) \cdot \\
&\quad \cdot \mu(\{\mathcal{N}(2(\bar{\Delta}_{bc}+t_B)+2t_B+(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}_{bc}+t_B))=0\})
\end{aligned} \tag{5.89}$$

$$\begin{aligned}
&\stackrel{(5.80)}{\geq} \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B}(G_{C,0} \cup G_{B;N_l^y-1;\bar{v}}) \cdot \\
&\quad \cdot \mu(\{\mathcal{N}((N_l^y-2)(\bar{\Delta}_{bc}+t_B))=0\}) \cdot \\
&\quad \cdot \mu(\{\mathcal{N}(2(\bar{\Delta}_{bc}+t_B)+2t_B+(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}_{bc}+t_B))=0\}) \\
&= \Pi_y^{(N_r^y+1)(\bar{\Delta}_{bc}+t_B)+t_B}(G_{C,0} \cup G_{B;N_l^y-1;\bar{v}}) \cdot \\
&\quad \cdot \mu(\{\mathcal{N}(N_l(\bar{\Delta}_{bc}+t_B)+2t_B+(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}_{bc}+t_B))=0\})
\end{aligned} \tag{5.90}$$

$$\begin{aligned}
&\stackrel{(5.84)}{\geq} \Pi_y^{N_r^y(\bar{\Delta}_{bc}+t_B)}(G_{C;N_l^y,0;\bar{v};2,-B})\mu(\{\mathcal{N}(\bar{\Delta}_{bc}+2t_B)=0\}) \cdot \\
&\quad \cdot \mu(\{\mathcal{N}(N_l(\bar{\Delta}_{bc}+t_B)+2t_B+(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}_{bc}+t_B))=0\}) \\
&= \Pi_y^{N_r^y(\bar{\Delta}_{bc}+t_B)}(G_{C;N_l^y,0;\bar{v};2,-B}) \cdot \\
&\quad \cdot \mu(\{\mathcal{N}((N_l+1)(\bar{\Delta}_{bc}+t_B)+3t_B+(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}_{bc}+t_B))=0\})
\end{aligned} \tag{5.91}$$

$$\begin{aligned}
&\stackrel{(5.85)}{\geq} \mu(\{\mathcal{N}(N_r^y(\bar{\Delta}_{bc}+t_B))=0\}) \cdot \\
&\quad \cdot \mu(\{\mathcal{N}((N_l+1)(\bar{\Delta}_{bc}+t_B)+3t_B+(\bar{N}-(N_r^y+N_l^y))(\bar{\Delta}_{bc}+t_B))=0\}) \\
&= \mu(\{\mathcal{N}((\bar{N}+1)(\bar{\Delta}_{bc}+t_B)+3t_B)=0\}).
\end{aligned} \tag{5.92}$$

Equalities (5.87), (5.88), (5.89), (5.90), (5.91), (5.92) follow by (2.7) and using (5.66) in a similar way which gave (5.67).

With that we can now end the proof of Lemma 5.4, since we have for the time in (5.86) that

$$\begin{aligned}
\bar{\Delta}_{\bar{N}} &\stackrel{(5.51)}{=} (\bar{N}+1)(\bar{\Delta}_{bc}+t_B)+3t_B \\
&\stackrel{(5.60)}{=} (\bar{N}+1) \left(\left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) + 3t_B \\
&\stackrel{(5.41)}{=} t(\bar{N})
\end{aligned}$$

and for (5.92)

$$\begin{aligned}
&\mu(\{\mathcal{N}((\bar{N}+1)(\bar{\Delta}_{bc}+t_B)+3t_B)=0\}) \\
&\stackrel{(5.22)}{=} \exp\left(-2\rho\left((\bar{N}+1)(\bar{\Delta}_{bc}+t_B)+3t_B\right)(\sqrt{2\pi\mathcal{K}m})^{-1}\right) \\
&= \exp\left(-2\rho(\bar{\Delta}_{bc}+4t_B)(\sqrt{2\pi\mathcal{K}m})^{-1}\right) \exp\left(-2\rho(\bar{\Delta}_{bc}+t_B)(\sqrt{2\pi\mathcal{K}m})^{-1}\bar{N}\right) \\
&\stackrel{(5.13),(5.60)}{=} \exp\left(-2\rho\left(\left(\rho \int_{D_b}^{D_c} v f(v) dv\right)^{-1} + 4t_B\right)(\sqrt{2\pi\mathcal{K}m})^{-1}\right).
\end{aligned}$$

$$\begin{aligned} & \cdot \exp \left(-2\rho \left(\left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) (\sqrt{2\pi\mathcal{K}m})^{-1} \bar{N} \right) \\ & = C_2 e^{-C_3 \bar{N}} \end{aligned}$$

with C_2, C_3 given in (5.43) resp. (5.44). \square

Recall that by Lemma 5.3 all states in $G_{\bar{V}, \bar{N}}$ (cf. (5.10)) can reach a state in $G_{B, \bar{N}; \bar{v}}$ (cf. (5.16)) or in $G_{B, \bar{V}; 0}$ (cf. (5.17)) by a certain time. If we now show how to proceed from $G_{B, \bar{V}; 0}$ to $G_{B, C; 0}$ (cf. (5.12)), we can proceed from any state in $G_{\bar{V}, \bar{N}}$ to $G_{B, C; 0}$, since in Lemma 5.4 we have already shown how to proceed from $G_{B, \bar{N}; \bar{v}}$ to $G_{B, C; 0}$.

Lemma 5.5. Let

$$\begin{aligned} t(\bar{V}) := & \frac{\bar{V}}{D_M B} \left(\left(2\rho \int_0^B v f(v) dv \right)^{-1} + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) + \\ & + 7t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \end{aligned} \quad (5.93)$$

with

$$D_M = \min \left\{ \frac{2m}{M+m}, \frac{2(M-m)}{M+m} \right\} \quad (5.94)$$

and D_b, D_c given in (5.25), t_B given in (5.13), then for any $y \in G_{B, \bar{V}; 0}$

$$\Pi_y^{t(\bar{V})}(G_{B, C; 0}) \geq C_4 e^{-C_5 \bar{V}} \quad (5.95)$$

with

$$C_4 := \exp \left(-\frac{2\rho}{\sqrt{2\pi\mathcal{K}m}} \left(7t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \right) \right) \quad (5.96)$$

$$C_5 := \frac{2\rho}{\sqrt{2\pi\mathcal{K}m}} \left(\left(2\rho \int_0^B v f(v) dv \right)^{-1} + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) \frac{1}{D_M B}. \quad (5.97)$$

Proof of Lemma 5.5. Recall that $G_{B, \bar{V}; 0}$ are all states where the molecule is alone in Λ with $B < |V| < \bar{V}$. Consider $\bar{V} \leq C$ (C given in (5.11)). Then,

$$G_{B, \bar{V}; 0} \subset G_{B, C; 0}. \quad (5.98)$$

Since the process starting in $G_{B, \bar{V}; 0}$ stays in $G_{B, \bar{V}; 0}$ as long as no atom enters Λ , we have

for $t > 0$ and $y \in G_{B,\bar{V};0}$ by (5.98) that

$$\Pi_y^t(G_{B,C;0}) \geq \mu(\{\mathcal{N}(t) = 0\}). \quad (5.99)$$

Lemma 5.5 then follows, since (5.99) holds for any $t > 0$, especially for $t(\bar{V})$ given in (5.93), and since

$$\begin{aligned} & \mu(\{\mathcal{N}(t(\bar{V})) = 0\}) \\ & \stackrel{(5.22),(5.93)}{=} \exp\left(-\frac{2\rho}{\sqrt{2\pi\mathcal{K}m}}\left(7t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv\right)^{-1}\right)\right) \\ & \quad \cdot \exp\left(-\frac{2\rho}{\sqrt{2\pi\mathcal{K}m}}\left(\left(2\rho \int_0^B v f(v) dv\right)^{-1} + \left(\rho \int_{D_b}^{D_c} v f(v) dv\right)^{-1} + t_B\right)\frac{\bar{V}}{D_{MB}}\right) \\ & \stackrel{(5.96),(5.97)}{=} C_4 e^{-C_5 \bar{V}}. \end{aligned} \quad (5.100)$$

Let now $\bar{V} > C$. We can write

$$G_{B,\bar{V};0} = G_{B,C;0} \cup G_{C,\bar{V};0}, \quad (5.101)$$

where

$$G_{C,\bar{V};0} := \{C < |V| < \bar{V}, N = 0\} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\} \quad (5.102)$$

is the set of configurations, where the molecule is alone in Λ with

$$C < |V| < \bar{V}.$$

To proceed from (5.101) to $G_{B,C;0}$, we distinguish in the following if the process starts in $G_{B,C;0}$ or in $G_{C,\bar{V};0}$.

First, consider $y \in G_{B,C;0}$. Since the process stays in $G_{B,C;0}$ as long as no atom enters Λ , we can estimate for any $t > 0$

$$\Pi_y^t(G_{B,C;0}) > \mu(\{\mathcal{N}(t) = 0\}). \quad (5.103)$$

Now consider $Y(0) = y \in G_{C,\bar{V};0}$. To obtain $Y(t) \in G_{B,C;0}$ for a time t , we have to slow down the molecule to $B < |V| < C$. There are various ways to slow down the molecule: If one sends in exactly one atom, then the velocity of this atom has to depend on V_0 , the velocity of the molecule at time $t = 0$, to cause $B < |V'| < C$, while if one sends in more than one atom, there are procedures where the number of atoms depends on V_0 but the velocities of the atoms may be chosen independent of it. The latter gives in Lemma 5.5 a time $t(\bar{V})$, which depends linearly on \bar{V} , while sending in one atom gives an exponential

dependency. The latter is based on the fact that the velocity of the atom is distributed according to the Maxwellian (cf. (2.5)). Since a time, which grows too fast with \bar{V} , may lead to a rate β (cf. (5.4)), which is not integrable, but integrability is one of the conditions of the fCLT (cf. (3.5)), we proceed from $G_{C,\bar{V};0}$ to $G_{B,C;0}$ by sending in a certain amount of atoms, whose velocities don't depend on V_0 .

Note, if one sends in atoms to slow down the molecule, some of these atoms may need to be pushed out afterwards so that the molecule is alone in Λ and the process reaches a state in $G_{B,C;0}$. Therefore, we proceed from $G_{C,\bar{V};0}$ to $G_{B,C;0}$ in several steps. In Step 1 we will slow down the molecule even to $|V| < B$, since then in Step 2 we can use the procedure described in the poof of Lemma 5.4 to push out the atoms and achieve the molecule alone in Λ with $B < |V| < C$.

Step 1: Let the molecule be alone in Λ with

$$C < |V_0| < \bar{V}. \quad (5.104)$$

To slow down the molecule to $|V| < B$, we send in atoms with

$$0 < |v| < B \quad (5.105)$$

and no others. Note following facts: If $|v| < |V|$, the velocity of the molecule and the atom have different signs when colliding. Further, as long as atoms with (5.105) collide with the molecule with $|V| > B$, they leave the interval without an additional collision, since $|v'| > |V'|$. The latter follows since $M > m$. If after some collisions the molecule is slowed down to $|V| < B$, but the molecule still collides with atoms with (5.105), the molecule stays slower than B , since $M > m$.

The larger $|V_0|$, the more atoms with (5.105) may be necessary to obtain $|V| < B$. Since $|V_0|$ is bounded by \bar{V} , there is an upper bound on the number of atoms with (5.105), which are needed to slow down the molecule to $|V| < B$. To specify this bound, we estimate how much the molecule is slowed down at least by a collision with an atom with velocity (5.105).

Let $V_i, i = 1, 2, \dots$ denote the velocity of the molecule after the collision with the i -th atom with pre collision velocity v_i , where the numbering is in respect to the order of collision.

Assertion 5.10. Let $V_{i-1} > B$ and $-B < v_i < 0$ or $V_{i-1} < -B$ and $0 < v_i < B$. Then,

$$|V_{i-1}| - |V_i| > D_M B$$

with D_M given in (5.94).

Poof of Assertion 5.10. First, we determine an upper bound for $|V_i|$ depending on $|V_{i-1}|$.

From the collision equation (2.1) we obtain the following. If $V_{i-1} > B$ and $-B < v_i < 0$, then

$$\frac{M-3m}{M+m}B < V_i < \frac{M-m}{M+m}V_{i-1}. \quad (5.106)$$

If $V_{i-1} < -B$ and $0 < v_i < B$, then

$$-\frac{M-m}{M+m}|V_{i-1}| < V_i < -\frac{M-3m}{M+m}B. \quad (5.107)$$

For $3m < M$ we have that

$$\frac{M-3m}{M+m}B > 0$$

and it follows that

$$\frac{M-3m}{M+m}B < |V_i| < \frac{M-m}{M+m}|V_{i-1}|.$$

For $2m < M \leq 3m$ we obtain

$$|V_i| < \frac{M-m}{M+m}|V_{i-1}|,$$

since

$$\frac{M-3m}{M+m}B \leq 0$$

but

$$-\frac{M-3m}{M+m}B < \frac{M-m}{M+m}|V_{i-1}|.$$

Hence, for $2m < M$ we may estimate the difference between $|V_{i-1}|$ and $|V_i|$ by

$$|V_{i-1}| - |V_i| > |V_{i-1}| - \frac{M-m}{M+m}|V_{i-1}| = \frac{2m}{M+m}|V_{i-1}| > \frac{2m}{M+m}B. \quad (5.108)$$

For $m < M \leq 2m$ there are values of V_{i-1} , namely

$$B < |V_{i-1}| < -\frac{M-3m}{M-m}B,$$

for which

$$-\frac{M-3m}{M+m}B > \frac{M-m}{M+m}|V_{i-1}|,$$

and values, namely

$$|V_{i-1}| \geq -\frac{M-3m}{M-m}B$$

for which

$$-\frac{M-3m}{M+m}B \leq \frac{M-m}{M+m}|V_{i-1}|,$$

so that with (5.106) and (5.107)

$$|V_i| < \max \left\{ -\frac{M-3m}{M+m}B, \frac{M-m}{M+m}|V_{i-1}| \right\}$$

and furthermore,

$$\begin{aligned} |V_{i-1}| - |V_i| &> |V_{i-1}| - \max \left\{ -\frac{M-3m}{M+m}B, \frac{M-m}{M+m}|V_{i-1}| \right\} \\ &= \min \left\{ |V_{i-1}| + \frac{M-3m}{M+m}B, \frac{2m}{M+m}|V_{i-1}| \right\} \\ &\stackrel{M \leq 2m}{>} \frac{2(M-m)}{M+m}B. \end{aligned} \tag{5.109}$$

All in all we have by (5.108) and (5.109) that

$$|V_{i-1}| - |V_i| > \min \left\{ \frac{2m}{M+m}, \frac{2(M-m)}{M+m} \right\} B.$$

Assertion 5.10 follows with (5.94). □

By Assertion 5.10 we can determine an upper bound on the number of atoms which are needed to obtain $|V| < B$: Let n such that $|V_{n-1}| > B$. Then, $|V_{i-1}| > B$ for any $i \in \{1, \dots, n\}$ and by Assertion 5.10 we get that

$$|V_0| - |V_n| = \sum_{i=1}^n |V_{i-1}| - |V_i| > \sum_{i=1}^n D_M B = nD_M B$$

and further,

$$|V_n| < -nD_M B + |V_0| \stackrel{|V_0| < \bar{V}}{<} -nD_M B + \bar{V}.$$

Since

$$-nD_M B + \bar{V} < B$$

$$\Leftrightarrow \frac{\bar{V}}{D_M B} - \frac{1}{D_M} < n, \quad (5.110)$$

for any $n \in \mathbb{N}$ with (5.110) it holds that $|V_n| < B$. Furthermore, there is exactly one $\tilde{n} \in \mathbb{N}$ with (5.110) such that

$$\frac{\bar{V}}{D_M B} - 1 < \tilde{n} \leq \frac{\bar{V}}{D_M B} =: \bar{n}_{\bar{V}}, \quad (5.111)$$

with D_M given in (5.94). Note, since $D_M < 1$, \tilde{n} with (5.111) fulfills indeed (5.110). That means if the molecule with (5.104) collides with \tilde{n} (or more) atoms with (5.105) (and no others) it will achieve $|V| < B$.

Now we specify the states in which the process is at a certain time if it starts in $G_{C, \bar{V}, 0}$ and if one sends in \tilde{n} atoms with (5.105) (and no others).

Consider $Y(0) = y \in G_{C, \bar{V}, 0}$ and let

$$\bar{\Delta} > 0. \quad (5.112)$$

Consider the event that \tilde{n} (cf. (5.111)) atoms with (5.105) (and no others) enter Λ during $[0, \bar{\Delta}]$ and no atom during $[\bar{\Delta}, \bar{\Delta} + 2t_B]$. Then, by time $\bar{\Delta} + 2t_B$ $|V| < B$. This follows since

- (i) if $|V(\bar{\Delta})| < B$: Once there is a j such that $|V_j| < B$, it follows that $|V_i| < B$ for $i \geq j$, since the remaining colliding atoms have velocity $0 < |v| < B$ and cannot make the molecule faster than B . Since $|V(\bar{\Delta})| < B$ it follows that $|V(t)| < B$ for $t \in [\bar{\Delta}, \bar{\Delta} + 2t_B]$;
- (ii) if $|V(\bar{\Delta})| \geq B$: Since \tilde{n} is a uniform upper bound on the number of atoms which are needed to achieve $|V| < B$, for any $y \in G_{C, \bar{V}, 0}$ there is a $n \leq \tilde{n}$ such that $|V_i| > B$ for $i \leq n - 1$ and $|V_n| < B$. Once $|V_n| < B$, it follows that $|V_i| < B$ for $i \geq n$, since the remaining colliding atoms have velocity $0 < |v| < B$ and cannot make the molecule faster than B . By time $\bar{\Delta}$ all \tilde{n} atoms have entered Λ . We know that by a collision with one of these atoms the molecule is slowed down from $|V| > B$ to a speed less than B . Let τ denote the time of this collision. Since $|V(t)| \geq B$ for all $t \in [\bar{\Delta}, \bar{\Delta} + \tau]$, the collision takes place before $\bar{\Delta} + 2t_B$.

Now we consider the event, that no atom enters Λ during $[\bar{\Delta} + 2t_B, \bar{\Delta} + 3t_B]$. We can conclude by a similar argumentation as in (a) underneath (5.14), that by time

$$\bar{\Delta} + 3t_B$$

there are no more than \tilde{n} atoms in Λ , each with

$$|v| < \frac{3M - m}{M + m} B =: \bar{v} \quad (5.113)$$

(cf. (5.15)).

By the above we can estimate transitions starting in $G_{C,\bar{V},0}$ and being at a certain time in $G_{B,\bar{n}_{\bar{V}},\bar{v}}$, where

$$G_{B,\bar{n}_{\bar{V}},\bar{v}} := \{|V| < B, N \leq \bar{n}_{\bar{V}}, |v| < \bar{v}\} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\} \quad (5.114)$$

is the set of configurations, where $|V| < B$, there are no more than $\bar{n}_{\bar{V}}$ (cf. (5.111)) atoms in Λ and each atom has velocity $|v| < \bar{v}$ (cf. (5.113)). We shall show that for any $y \in G_{C,\bar{V},0}$ and

$$t_1(\bar{V}) := \frac{\bar{n}_{\bar{V}}}{2\rho \int_0^B v f(v) dv} + 3t_B \quad (5.115)$$

with t_B given in (5.13), we have that

$$\Pi_y^{t_1(\bar{V})}(G_{B,\bar{n}_{\bar{V}},\bar{v}}) \geq \mu(\{\mathcal{N}(t_1(\bar{V})) = 0\}). \quad (5.116)$$

To prove (5.116) consider $Y(0) = y \in G_{C,\bar{V},0}$, i.e. the molecule is alone in Λ with $C < |V| < \bar{V}$. Let $\bar{\Delta}$ as given in (5.112). Since \mathcal{M}_t is a stationary Markov process

$$\Pi_y^{\bar{\Delta}+3t_B}(G_{B,\bar{n}_{\bar{V}},\bar{v}}) = \int \Pi_y^{\bar{\Delta}}(dy') \Pi_{y'}^{3t_B}(G_{B,\bar{n}_{\bar{V}},\bar{v}}). \quad (5.117)$$

To continue estimating (5.117), denote by $H \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ the set of configurations, which are possible for the system at time $\bar{\Delta}$, starting in $G_{C,\bar{V},0}$ and undergoing the procedure we described underneath (5.112), i.e. with ease of notation

$$\begin{aligned} H = & \{|V| < B \text{ and there are no more than } \tilde{n} \text{ atoms in } \Lambda. \\ & \text{If for an atom } |v| > B, \\ & \text{then it moves in opposite direction of the molecule.} \} \\ \cup & \{|V| > B, \text{ and there are no more than } \tilde{n} \text{ atoms in } \Lambda. \\ & \text{If for an atom } |v| > B, \\ & \text{then it moves in opposite direction of the molecule.} \\ & \text{If } 0 < |v| < B, \text{ the atom moves towards the molecule.} \\ & \text{By at least one of the collision with these atoms, } |V'| < B. \} \end{aligned}$$

with \tilde{n} given in (5.111). We then have

$$(5.117) \geq \int_H \Pi_y^{\bar{\Delta}}(dy') \Pi_{y'}^{3t_B}(G_{B,\bar{n}_{\bar{V}},\bar{v}}). \quad (5.118)$$

By arguments (i) and (ii) we gave above and by similar argumentation as in (a) underneath

(5.14), for any $Y(0) = y' \in H$ we have that $Y(3t_B) \in G_{B, \bar{n}_{\bar{v}}, \bar{v}}$ if no atom enters Λ during $[0, 3t_B]$. With that we get that

$$\begin{aligned} (5.118) &\geq \int_H \Pi_y^{\bar{\Delta}}(dy') \mu(\{\mathcal{N}(3t_B) = 0\}) \\ &= \Pi_y^{\bar{\Delta}}(H) \mu(\{\mathcal{N}(3t_B) = 0\}). \end{aligned} \quad (5.119)$$

By definition of H , for $Y(0) = y \in G_{C, \bar{v}, 0}$ we have that $Y(\bar{\Delta}) = y \in H$ if \tilde{n} atoms with (5.105) (and no others) enter Λ during $[0, \bar{\Delta}]$. Hence, it follows that

$$\Pi_y^{\bar{\Delta}}(H) \geq \mu(\{\mathcal{N}_{|0, B|}(\bar{\Delta}) = \tilde{n}\}) \mu(\{\mathcal{N}_{|B, \infty|}(\bar{\Delta}) = 0\}). \quad (5.120)$$

Until now $\bar{\Delta}$ can be any time > 0 (cf. (5.112)). To estimate the r.h.s. of (5.120) by $\mu(\{\mathcal{N}(\bar{\Delta}) = 0\})$, so that we obtain at the end an estimation similar to (5.116), we need to specify $\bar{\Delta}$. Since $\mathcal{N}_{|0, B|}(\bar{\Delta})$, the number of atoms with $0 < |v| < B$ entering Λ in a time interval of length $\bar{\Delta}$, is a Poisson random variable with

$$\mathbb{E}(\mathcal{N}_{|0, B|}(\bar{\Delta})) = \bar{\Delta} 2\rho \int_0^B v f(v) dv,$$

it follows that in a time interval of length

$$\bar{\Delta}_{\bar{v}} := \frac{\bar{n}_{\bar{v}}}{2\rho \int_0^B v f(v) dv} \quad (5.121)$$

($\bar{n}_{\bar{v}}$ given in (5.111)) the expected number of atoms entering with $0 < |v| < B$ is

$$\mathbb{E}(\mathcal{N}_{|0, B|}(\bar{\Delta}_{\bar{v}})) = \bar{n}_{\bar{v}}. \quad (5.122)$$

Choosing

$$\bar{\Delta} = \bar{\Delta}_{\bar{v}}$$

and using the monotonicity of Poisson random variables (cf. (5.62)) for the random variable $\mathcal{N}_{|0, B|}(\bar{\Delta}_{\bar{v}})$ with mean $\bar{n}_{\bar{v}}$ (cf. (5.122)), we can estimate since $\bar{n}_{\bar{v}} \geq \tilde{n} > 0$

$$\begin{aligned} (5.120) &\stackrel{(5.62)}{\geq} \mu(\{\mathcal{N}_{|0, B|}(\bar{\Delta}_{\bar{v}}) = 0\}) \mu(\{\mathcal{N}_{|B, \infty|}(\bar{\Delta}_{\bar{v}}) = 0\}) \\ &\stackrel{(2.7)}{=} \mu(\{\mathcal{N}(\bar{\Delta}_{\bar{v}}) = 0\}). \end{aligned} \quad (5.123)$$

Finally, (5.116) follows since for (5.117) from (5.118), (5.119), (5.120) and (5.123) we have for $y \in G_{C, \bar{v}, 0}$ that

$$\Pi_y^{\bar{\Delta}_{\bar{v}} + 3t_B}(G_{B, \bar{n}_{\bar{v}}, \bar{v}}) \geq \mu(\{\mathcal{N}(\bar{\Delta}_{\bar{v}} + 3t_B) = 0\}),$$

with

$$\bar{\Delta}_{\bar{V}} + 3t_B \stackrel{(5.115),(5.121)}{=} t_1(\bar{V}).$$

Step 2: Recall that in Lemma 5.5 we have as target set $G_{B,C;0}$ (cf. (5.12)), so now we need to proceed from $G_{B,\bar{n}_{\bar{V}},\bar{v}}$ (cf. (5.114)) to $G_{B,C;0}$. We immediately obtain an estimate for the transitions starting in $G_{B,\bar{n}_{\bar{V}},\bar{v}}$ since we can use Lemma 5.4. (Note that $\tilde{v} = \bar{v}$ (cf. (5.16), (5.113))): For

$$t_2(\bar{n}_{\bar{V}}) := (\bar{n}_{\bar{V}} + 1) \left(\left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) + 3t_B \quad (5.124)$$

with $\bar{n}_{\bar{V}}$ given in (5.111), D_b, D_c given in (5.25), t_B given in (5.13),

$$\Pi_y^{t_2(\bar{n}_{\bar{V}})}(G_{B,C;0}) \geq \mu(\{\mathcal{N}(t_2(\bar{n}_{\bar{V}})) = 0\}) \quad (5.125)$$

for any $y \in G_{B,\bar{n}_{\bar{V}},\bar{v}}$.

In Step 1 and Step 2 we have shown how to proceed from $G_{C,\bar{V};0}$ (cf. (5.102)) to $G_{B,\bar{n}_{\bar{V}},\bar{v}}$ (cf. (5.114)) and from $G_{B,\bar{n}_{\bar{V}},\bar{v}}$ to $G_{B,C;0}$ (cf. (5.12)) and we obtain by these steps, since \mathcal{M}_t is a stationary Markov process, for $y \in G_{C,\bar{V};0}$ that

$$\begin{aligned} \Pi_y^{t_1(\bar{V})+t_2(\bar{n}_{\bar{V}})}(G_{B,C;0}) &= \int \Pi_y^{t_1(\bar{V})}(dy') \Pi_{y'}^{t_2(\bar{n}_{\bar{V}})}(G_{B,C;0}) \quad (5.126) \\ &\geq \int_{G_{B,\bar{n}_{\bar{V}},\bar{v}}} \Pi_y^{t_1(\bar{V})}(dy') \Pi_{y'}^{t_2(\bar{n}_{\bar{V}})}(G_{B,C;0}) \\ &\stackrel{(5.125)}{\geq} \int_{G_{B,\bar{n}_{\bar{V}},\bar{v}}} \Pi_y^{t_1(\bar{V})}(dy') \mu(\{\mathcal{N}(t_2(\bar{n}_{\bar{V}})) = 0\}) \\ &= \Pi_y^{t_1(\bar{V})}(G_{B,\bar{n}_{\bar{V}},\bar{v}}) \mu(\{\mathcal{N}(t_2(\bar{n}_{\bar{V}})) = 0\}) \\ &\stackrel{(5.116)}{\geq} \mu(\{\mathcal{N}(t_1(\bar{V})) = 0\}) \mu(\{\mathcal{N}(t_2(\bar{n}_{\bar{V}})) = 0\}) \\ &\stackrel{(2.7)}{=} \mu(\{\mathcal{N}(t_1(\bar{V}) + t_2(\bar{n}_{\bar{V}})) = 0\}) \quad (5.127) \end{aligned}$$

with $t_1(\bar{V})$ given in (5.115), $t_2(\bar{n}_{\bar{V}})$ given in (5.124). With that we can end the proof of Lemma 5.5 for $\bar{V} > C$: Since

$$\begin{aligned} t_1(\bar{V}) + t_2(\bar{n}_{\bar{V}}) &= \\ &\stackrel{(5.115),(5.124)}{=} \frac{\bar{n}_{\bar{V}}}{2\rho \int_0^B v f(v) dv} + 3t_B + (\bar{n}_{\bar{V}} + 1) \left(\left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) + 3t_B \\ &\stackrel{(5.111)}{=} \frac{\bar{V}}{D_{MB}} \frac{1}{2\rho \int_0^B v f(v) dv} + \left(\frac{\bar{V}}{D_{MB}} + 1 \right) \left(\left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) + 6t_B \end{aligned}$$

$$\stackrel{(5.93)}{=} t(\bar{V})$$

it follows for (5.126) with (5.127) that

$$\Pi_y^{t_1(\bar{V})+t_2(\bar{n}_{\bar{V}})}(G_{B,C;0}) = \Pi_y^{t(\bar{V})}(G_{B,C;0}) \geq \mu(\{\mathcal{N}(t(\bar{V})) = 0\}) \quad (5.128)$$

for any $y \in G_{C,\bar{V};0}$.

Since (5.103) is valid for $y \in G_{B,C;0}$ and any $t > 0$, especially for $t(\bar{V})$ (cf. (5.93)), we obtain by (5.103) and (5.128) with (5.100) that for any $y \in G_{B,C;0} \cup G_{C,\bar{V};0} \stackrel{(5.101)}{=} G_{B,\bar{V};0}$ that

$$\Pi_y^{t(\bar{V})}(G_{B,C;0}) \geq C_4 e^{-C_5 \bar{V}}.$$

□

Taking Lemma 5.3, Lemma 5.4 and Lemma 5.5 together, we get estimates for transitions, which start in $G_{\bar{V},\bar{N}}$ (cf. (5.10)) and reach states in $G_{B,C;0}$ (cf. (5.12)) at a certain time. We can show now the following lemma, which we need for the proof of the Overlap-Lemma 5.2.

Lemma 5.6. Let

$$t(\bar{V}, \bar{N}) := \max\{4t_B + t(\bar{V}), 4t_B + t(\bar{N})\} \quad (5.129)$$

with t_B given in (5.13), $t(\bar{V})$ given in (5.93) and $t(\bar{N})$ given in (5.41), then for any $y \in G_{\bar{V},\bar{N}}$

$$\Pi_y^{t(\bar{V},\bar{N})}(G_{B,C;0}) \geq \varepsilon(\bar{V}, \bar{N}) \quad (5.130)$$

with

$$\varepsilon(\bar{V}, \bar{N}) := \min\{C_1 C_4 e^{-C_5 \bar{V}}, C_1 C_2 e^{-C_3 \bar{N}}\} \cdot \min\{C_{10} e^{-C_{11} \bar{V}}, C_{12} e^{-C_{13} \bar{N}}\} \quad (5.131)$$

with C_1 given in (5.18), C_2, C_3 given in (5.43) resp. (5.44), C_4, C_5 given in (5.96) resp. (5.97) and

$$C_{10} := \exp\left(-4\rho \left(11t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv\right)^{-1}\right) (\sqrt{2\pi\mathcal{K}m})^{-1}\right), \quad (5.132)$$

$$C_{11} := \frac{4\rho}{D_M B} \left(t_B + \left(2\rho \int_0^B v f(v) dv\right)^{-1} + \left(\rho \int_{D_b}^{D_c} v f(v) dv\right)^{-1}\right) (\sqrt{2\pi\mathcal{K}m})^{-1} \quad (5.133)$$

$$C_{12} := \exp \left(-4\rho \left(8t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \right) \left(\sqrt{2\pi\mathcal{K}m} \right)^{-1} \right), \quad (5.134)$$

$$C_{13} := 4\rho \left(t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \right) \left(\sqrt{2\pi\mathcal{K}m} \right)^{-1} \quad (5.135)$$

with D_b, D_c given in (5.25) and D_M given in (5.94).

Proof of Lemma 5.6. Note, since \mathcal{M}_t is a stationary Markov process, we obtain by Lemma 5.3 and Lemma 5.4 resp. Lemma 5.5, for $y \in G_{\bar{V}, \bar{N}}$ (cf. (5.10)) that either

(i) if $\Pi_y^{4t_B}(G_{B; \bar{N}; \bar{v}}) \geq C_1$, then

$$\begin{aligned} \Pi_y^{4t_B+t(\bar{N})}(G_{B,C;0}) &= \int \Pi_y^{4t_B}(dy') \Pi_{y'}^{t(\bar{N})}(G_{B,C;0}) \\ &\geq \int_{G_{B; \bar{N}; \bar{v}}} \Pi_y^{4t_B}(dy') \Pi_{y'}^{t(\bar{N})}(G_{B,C;0}) \\ &\stackrel{(5.42)}{\geq} \int_{G_{B; \bar{N}; \bar{v}}} \Pi_y^{4t_B}(dy') C_2 e^{-C_3 \bar{N}} \\ &= \Pi_y^{4t_B}(G_{B; \bar{N}; \bar{v}}) C_2 e^{-C_3 \bar{N}} \\ &\stackrel{(5.19)}{\geq} C_1 C_2 e^{-C_3 \bar{N}} \end{aligned} \quad (5.136)$$

with $G_{B; \bar{N}; \bar{v}}$ given in (5.16), $t(\bar{N})$ given in (5.41), C_1 given in (5.18) and C_2, C_3 given in (5.43) resp. (5.44),

or

(ii) if $\Pi_y^{4t_B}(G_{B; \bar{V}; 0}) \geq C_1$, then

$$\begin{aligned} \Pi_y^{4t_B+t(\bar{V})}(G_{B,C;0}) &= \int \Pi_y^{4t_B}(dy') \Pi_{y'}^{t(\bar{V})}(G_{B,C;0}) \\ &\geq \int_{G_{B; \bar{V}; 0}} \Pi_y^{4t_B}(dy') \Pi_{y'}^{t(\bar{V})}(G_{B,C;0}) \\ &\stackrel{(5.95)}{\geq} \int_{G_{B; \bar{V}; 0}} \Pi_y^{4t_B}(dy') C_4 e^{-C_5 \bar{V}} \\ &= \Pi_y^{4t_B}(G_{B; \bar{V}; 0}) C_4 e^{-C_5 \bar{V}} \\ &\stackrel{(5.20)}{\geq} C_1 C_4 e^{-C_5 \bar{V}} \end{aligned} \quad (5.137)$$

with $G_{B; \bar{V}; 0}$ given in (5.17), $t(\bar{V})$ given in (5.93), C_1 given in (5.18), C_4, C_5 given in (5.96) resp. (5.97).

We now estimate

$$\Pi_y^{t(\bar{V}, \bar{N})}(G_{B,C;0})$$

to show Lemma 5.6 by using estimates (5.136) and (5.137). Recall that

$$t(\bar{V}, \bar{N}) \stackrel{(5.129)}{=} \max\{4t_B + t(\bar{V}), 4t_B + t(\bar{N})\}.$$

We first give separate estimates depending on the value of $t(\bar{V}, \bar{N})$, i.e. we distinguish if $t(\bar{V}, \bar{N}) = 4t_B + t(\bar{N})$ or if $t(\bar{V}, \bar{N}) = 4t_B + t(\bar{V})$. Within these cases we distinguish a second time, namely as in (5.136) and (5.137).

Set

$$t_{\bar{V}} := 4t_B + t(\bar{V}) \tag{5.138}$$

$$\begin{aligned} &\stackrel{(5.93)}{=} \frac{\bar{V}}{D_M B} \left(\left(2\rho \int_0^B v f(v) dv \right)^{-1} + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) + \\ &\quad + 11t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \\ &= C_6 + C_7 \bar{V} \end{aligned} \tag{5.139}$$

with

$$C_6 := 11t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1}, \tag{5.140}$$

and

$$C_7 := \frac{1}{D_M B} \left(\left(2\rho \int_0^B v f(v) dv \right)^{-1} + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) \tag{5.141}$$

with D_b, D_c given in (5.25) and D_M given in (5.94), and set

$$t_{\bar{N}} := 4t_B + t(\bar{N}) \tag{5.142}$$

$$\begin{aligned} &\stackrel{(5.41)}{=} (\bar{N} + 1) \left(\left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + t_B \right) + 7t_B \\ &= C_8 + C_9 \bar{N} \end{aligned} \tag{5.143}$$

with

$$C_8 := 8t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1}, \tag{5.144}$$

and

$$C_9 := t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \quad (5.145)$$

with D_b, D_c given in (5.25).

Assume $t(\bar{V}, \bar{N}) = t_{\bar{N}}$, then

(i) if $\Pi_y^{4t_B}(G_{B;\bar{N};\bar{v}}) \geq C_1$, we have

$$\begin{aligned} \Pi_y^{t(\bar{V}, \bar{N})}(G_{B,C;0}) &= \Pi_y^{t_{\bar{N}}}(G_{B,C;0}) \\ &\stackrel{(5.142)}{=} \Pi_y^{4t_B+t(\bar{N})}(G_{B,C;0}) \\ &\stackrel{(5.136)}{\geq} C_1 C_2 e^{-C_3 \bar{N}}, \end{aligned} \quad (5.146)$$

(ii) if $\Pi_y^{4t_B}(G_{B;\bar{V};0}) \geq C_1$, we have that

$$\begin{aligned} \Pi_y^{t(\bar{V}, \bar{N})}(G_{B,C;0}) &= \Pi_y^{t_{\bar{N}}}(G_{B,C;0}) \\ &= \Pi_y^{t_{\bar{V}}+(t_{\bar{N}}-t_{\bar{V}})}(G_{B,C;0}) \\ &= \int \Pi_y^{t_{\bar{V}}}(\mathrm{d}y') \Pi_{y'}^{t_{\bar{N}}-t_{\bar{V}}}(G_{B,C;0}) \\ &\geq \int_{G_{B,C;0}} \Pi_y^{t_{\bar{V}}}(\mathrm{d}y') \Pi_{y'}^{t_{\bar{N}}-t_{\bar{V}}}(G_{B,C;0}). \end{aligned} \quad (5.147)$$

Since $Y(0) = y' \in G_{B,C;0}$ stays in $G_{B,C;0}$ until $t_{\bar{N}} - t_{\bar{V}}$ if no atom enters Λ during $[0, t_{\bar{N}} - t_{\bar{V}}]$, we can estimate (5.147) as follows.

$$\begin{aligned} &\int_{G_{B,C;0}} \Pi_y^{t_{\bar{V}}}(\mathrm{d}y') \Pi_{y'}^{t_{\bar{N}}-t_{\bar{V}}}(G_{B,C;0}) \\ &\geq \int_{G_{B,C;0}} \Pi_y^{t_{\bar{V}}}(\mathrm{d}y') \mu(\{\mathcal{N}(t_{\bar{N}} - t_{\bar{V}}) = 0\}) \\ &\stackrel{(5.138)}{=} \Pi_y^{4t_B+t(\bar{V})}(G_{B,C;0}) \mu(\{\mathcal{N}(t_{\bar{N}} - t_{\bar{V}}) = 0\}) \\ &\stackrel{(5.137)}{\geq} C_1 C_4 e^{-C_3 \bar{V}} \mu(\{\mathcal{N}(t_{\bar{N}} - t_{\bar{V}}) = 0\}). \end{aligned} \quad (5.148)$$

Assume now $t(\bar{V}, \bar{N}) = t_{\bar{V}}$, then

(i) if $\Pi_y^{4t_B}(G_{B;\bar{N};\bar{v}}) \geq C_1$, we have

$$\begin{aligned} \Pi_y^{t(\bar{V}, \bar{N})}(G_{B,C;0}) &= \Pi_y^{t_{\bar{V}}}(G_{B,C;0}) \\ &= \Pi_y^{t_{\bar{N}}+(t_{\bar{V}}-t_{\bar{N}})}(G_{B,C;0}) \\ &= \int \Pi_y^{t_{\bar{N}}}(\mathrm{d}y') \Pi_{y'}^{t_{\bar{V}}-t_{\bar{N}}}(G_{B,C;0}) \end{aligned}$$

$$\geq \int_{G_{B,C;0}} \Pi_y^{t_{\bar{N}}}(\mathrm{d}y') \Pi_{y'}^{t_{\bar{V}}-t_{\bar{N}}}(G_{B,C;0}). \quad (5.149)$$

Since $Y(0) = y' \in G_{B,C;0}$ stays in $G_{B,C;0}$ until $t_{\bar{V}} - t_{\bar{N}}$ if no atom enters Λ during $[0, t_{\bar{V}} - t_{\bar{N}}]$, we get for (5.149)

$$\begin{aligned} & \int_{G_{B,C;0}} \Pi_y^{t_{\bar{N}}}(\mathrm{d}y') \Pi_{y'}^{t_{\bar{V}}-t_{\bar{N}}}(G_{B,C;0}) \\ & \geq \int_{G_{B,C;0}} \Pi_y^{t_{\bar{N}}}(\mathrm{d}y') \mu(\{\mathcal{N}(t_{\bar{V}} - t_{\bar{N}}) = 0\}) \\ & \stackrel{(5.142)}{=} \Pi_y^{4t_B+t(\bar{N})}(G_{B,C;0}) \mu(\{\mathcal{N}(t_{\bar{V}} - t_{\bar{N}}) = 0\}) \\ & \stackrel{(5.136)}{\geq} C_1 C_2 e^{-C_3 \bar{N}} \mu(\{\mathcal{N}(t_{\bar{V}} - t_{\bar{N}}) = 0\}) \end{aligned} \quad (5.150)$$

(ii) if $\Pi_y^{4t_B}(G_{B;\bar{V};0}) \geq C_1$, we have that

$$\begin{aligned} \Pi_y^{t(\bar{V}, \bar{N})}(G_{B,C;0}) &= \Pi_y^{t_{\bar{V}}}(G_{B,C;0}) \\ & \stackrel{(5.138)}{=} \Pi_y^{4t_B+t(\bar{V})}(G_{B,C;0}) \\ & \stackrel{(5.137)}{\geq} C_1 C_4 e^{-C_5 \bar{V}}. \end{aligned} \quad (5.151)$$

Combining all four estimates (5.146), (5.148), (5.150), (5.151) we obtain, since

$$\mu(\{\mathcal{N}(|t_{\bar{N}} - t_{\bar{V}}|) = 0\}) < 1,$$

that

$$\begin{aligned} \Pi_y^{t(\bar{V}, \bar{N})}(G_{B,C;0}) &\geq \min \left\{ C_1 C_2 e^{-C_3 \bar{N}}, C_1 C_4 e^{-C_5 \bar{V}} \right\} \\ &\quad \cdot \mu(\{\mathcal{N}(|t_{\bar{V}} - t_{\bar{N}}|) = 0\}) \end{aligned} \quad (5.152)$$

with

$$\mu(\{\mathcal{N}(|t_{\bar{V}} - t_{\bar{N}}|) = 0\}) \stackrel{(5.22)}{=} \exp \left(-\frac{2\rho |t_{\bar{V}} - t_{\bar{N}}|}{\sqrt{2\pi \mathcal{K} m}} \right). \quad (5.153)$$

Since $|t_{\bar{V}} - t_{\bar{N}}| \leq 2 \cdot \max \{t_{\bar{V}}, t_{\bar{N}}\}$ it follows for (5.153) that

$$\begin{aligned} & \mu(\{\mathcal{N}(|t_{\bar{V}} - t_{\bar{N}}|) = 0\}) = \\ & = \exp \left(-\frac{2\rho |t_{\bar{V}} - t_{\bar{N}}|}{\sqrt{2\pi \mathcal{K} m}} \right) \\ & \geq \min \left\{ \exp \left(-\frac{4\rho t_{\bar{V}}}{\sqrt{2\pi \mathcal{K} m}} \right), \exp \left(-\frac{4\rho t_{\bar{N}}}{\sqrt{2\pi \mathcal{K} m}} \right) \right\} \end{aligned} \quad (5.154)$$

$$\stackrel{(5.139)(5.143)}{=} \min \left\{ \exp \left(-\frac{4\rho(C_6 + C_7\bar{V})}{\sqrt{2\pi\mathcal{K}m}} \right), \exp \left(-\frac{4\rho(C_8 + C_9\bar{N})}{\sqrt{2\pi\mathcal{K}m}} \right) \right\}. \quad (5.155)$$

We now show that (5.155) is an equivalent expression of the second factor in (5.131). With

$$\exp \left(-\frac{4\rho C_6}{\sqrt{2\pi\mathcal{K}m}} \right) \stackrel{(5.140)}{=} \exp \left(-\frac{4\rho \left(11t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \right)}{\sqrt{2\pi\mathcal{K}m}} \right) \stackrel{(5.132)}{=} C_{10}$$

and

$$\begin{aligned} \frac{4\rho C_7}{\sqrt{2\pi\mathcal{K}m}} &\stackrel{(5.141)}{=} \frac{1}{D_M B} \left(\frac{1}{2\rho \int_0^B v f(v) dv} + \frac{1}{\rho \int_{D_b}^{D_c} v f(v) dv} + t_B \right) \frac{4\rho}{\sqrt{2\pi\mathcal{K}m}} \\ &\stackrel{(5.133)}{=} C_{11}, \end{aligned}$$

we have that

$$\exp \left(-\frac{4\rho(C_6 + C_7\bar{V})}{\sqrt{2\pi\mathcal{K}m}} \right) = C_{10} e^{-C_{11}\bar{V}}, \quad (5.156)$$

and with

$$\exp \left(-\frac{4\rho C_8}{\sqrt{2\pi\mathcal{K}m}} \right) \stackrel{(5.144)}{=} \exp \left(-\frac{4\rho \left(8t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \right)}{\sqrt{2\pi\mathcal{K}m}} \right) \stackrel{(5.134)}{=} C_{12}$$

and

$$\frac{4\rho C_9}{\sqrt{2\pi\mathcal{K}m}} \stackrel{(5.145)}{=} \frac{4\rho \left(t_B + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \right)}{\sqrt{2\pi\mathcal{K}m}} \stackrel{(5.135)}{=} C_{13},$$

we have that

$$\exp \left(-\frac{4\rho(C_8 + C_9\bar{N})}{\sqrt{2\pi\mathcal{K}m}} \right) = C_{12} e^{-C_{13}\bar{N}}. \quad (5.157)$$

Plugging (5.156) and (5.157) into (5.155) we obtain for (5.154) that

$$\mu(\{\mathcal{N}(|t_{\bar{V}} - t_{\bar{N}}|) = 0\}) \geq \min \left\{ C_{10} e^{-C_{11}\bar{V}}, C_{12} e^{-C_{13}\bar{N}} \right\}. \quad (5.158)$$

Finally, Lemma 5.6 follows, since with (5.158) we obtain for (5.152) that

$$\Pi_y^{t(\bar{V}, \bar{N})}(G_{B,C;0}) \geq \min \left\{ C_1 C_4 e^{-C_5\bar{V}}, C_1 C_2 e^{-C_3\bar{N}} \right\} \min \left\{ C_{10} e^{-C_{11}\bar{V}}, C_{12} e^{-C_{13}\bar{N}} \right\}$$

$$\stackrel{(5.131)}{=} \varepsilon(\bar{V}, \bar{N})$$

for any $y \in G_{\bar{V}, \bar{N}}$. □

The last remaining step we need for the proof of the Overlap-Lemma 5.2, is to establish overlap of transitions starting in $G_{B,C;0}$ (cf. (5.12)). We specify an explicit set, the overlap set, where loosely speaking any state can be reached at a certain time by a positive probability starting in any state in $G_{B,C;0}$. Proving that, we let atoms enter Λ depending on the molecular velocity and position as well as the value of σ (cf. (2.14)). To keep it simple, we choose the overlap set such, that the molecule is alone, and that any state in the overlap set can be reached by any starting state in $G_{B,C;0}$ by sending in exactly one atom, which leaves by time the interval again. By identifying the overlap set one has to take care of “virtual collisions”. These are collisions which are impossible if one knows the past trajectory of the molecule. Since these depend on the mass of the molecule M and hence, on the overlap set as well, we distinguish in the following different cases depending on M , namely if $M > 3m$, $3m \geq M > 2m$ or $2m \geq M > m$.

Denote by \mathbb{P} the path measure induced by \mathcal{M}_t and let \mathbb{P}_y denote the conditional path measure given $Y(0) = y$, $y \in \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$. Consider $Y(0) = y \in G_{B,C;0}$.

Case $M > 3m$

Denote by τ_1 the time when the molecule hits the wall at L the first time after $t = 0$, and by τ_2 the time when the molecule hits the wall at L the next time after τ_1 . Define $V_1 := V(\tau_1)$, $\sigma_1 := \sigma(\tau_1)$ and $V_2 := V(\tau_2)$, $\sigma_2 := \sigma(\tau_2)$.

Lemma 5.7. Let $Y(0) = y \in G_{B,C;0}$. Denote by O the set of paths with

$$O := \left\{ \text{Molecule is alone at time } \tau_2, \right. \tag{5.159}$$

$$V_2 \in \mathcal{V}_2 := \left(-\frac{M-3m}{M+m} \frac{B}{5}, -\frac{M-3m}{M+3m} \frac{B}{5} \right), \tag{5.160}$$

$$\tau_2 \in \mathcal{T}_2 := \left(\frac{10L}{B} \frac{M}{M-3m}, \frac{10L}{B} \frac{M+m}{M-3m} \right), \tag{5.161}$$

$$\sigma_2 = 1 \left. \right\}.$$

Then, there is a function $h_y : \mathcal{V}_2 \times \mathcal{T}_2 \rightarrow \mathbb{R}^+$ such that

$$\mathbb{P}_y(dY) \geq h_y(V_2, \tau_2) dV_2 d\tau_2 \tag{5.162}$$

for $dY \subset O$ with $Y(\tau_2) = (L, V_2, \sigma_2)$.

Furthermore there is a constant $g > 0$, which will be specified later, such that

$$h_y \geq g \tag{5.163}$$

for any $y \in G_{B,C;0}$.

Proof of Lemma 5.7. Consider $Y(0) = y \in G_{B,C;0}$, i.e.

$$y = (Q_0, V_0, \sigma_0) \tag{5.164}$$

with $B < |V_0| < C$. Denote by $\tau_1(y)$ the value of τ_1 for the process with $Y(0) = y$. If the molecule moves freely in Λ , then $\tau_1(y)$ with (5.164) is given by

$$\tau_1(y) = \begin{cases} \frac{L-Q_0}{V_0} & , V_0 > 0 \\ \frac{3L+Q_0}{|V_0|} & , V_0 < 0 \end{cases} \tag{5.165}$$

with

$$0 < \tau_1(y) \leq 2t_B, \tag{5.166}$$

and t_B given in (5.13). Inequality (5.166) follows, since $B < |V_0| < C$. Consider the event $\mathcal{E}_{\tau_1(y)} \subset \hat{\Omega}$ with

$$\mathcal{E}_{\tau_1(y)} := \{\text{No atom enters } \Lambda \text{ during } [0, \tau_1(y)]\}. \tag{5.167}$$

Then, at time $\tau_1(y)$ the molecule is alone in the interval and

$$Y(\tau_1(y)) = (L, V_1, \sigma_1), \tag{5.168}$$

with

$$V_1 = \begin{cases} -V_0 & , V_0 > 0 \\ V_0 & , V_0 < 0 \end{cases}, \tag{5.169}$$

$$\sigma_1 = \begin{cases} -\sigma_0 & , V_0 > 0 \\ \sigma_0 & , V_0 < 0 \end{cases}. \tag{5.170}$$

Note that

$$-C \leq V_1 \leq -B, \tag{5.171}$$

with C given in (5.11).

Denote by $\mathcal{C}_y(\mathcal{E}_{\tau_1(y)})$ the corresponding set of paths of \mathcal{M}_t to $\{Y(0) = y, \mathcal{E}_{\tau_1(y)}\}$, i.e. the set of all paths of \mathcal{M}_t for which $Y(0) = y$ and $\mathcal{E}_{\tau_1(y)}$ is possible. Then, we have for y given

in (5.164) that

$$\mathbb{P}_y(dY(\cdot + \tau_1(y))) \geq \mathbb{P}_y(dY(\cdot + \tau_1(y)) \cap \mathcal{C}_y(\mathcal{E}_{\tau_1(y)})) \quad (5.172)$$

$$= \mathbb{P}(dY(\cdot + \tau_1(y)) | \mathcal{C}_y(\mathcal{E}_{\tau_1(y)})) \mathbb{P}_y(\mathcal{C}_y(\mathcal{E}_{\tau_1(y)})). \quad (5.173)$$

Note that $\mathcal{C}_y(\mathcal{E}_{\tau_1(y)})$ exists of exactly one path, and the trajectory of this path is determined until time $\tau_1(y)$. Denote by $\{Y(0) = y; Y(t), t \leq \tau_1(y)\}$ the trajectory of this path, then we obtain that

$$\begin{aligned} & \mathbb{P}(dY(\cdot + \tau_1(y)) | \mathcal{C}_y(\mathcal{E}_{\tau_1(y)})) \\ &= \mathbb{P}(dY(\cdot + \tau_1(y)) | \{Y(0) = y; Y(t), t \leq \tau_1(y)\}) \\ &= \mathbb{P}(dY(\cdot + \tau_1(y)) | Y(\tau_1(y))) \end{aligned} \quad (5.174)$$

with $Y(\tau_1(y))$ given in (5.168). Note that (5.174) follows by the Markov property. With

$$\begin{aligned} \mathbb{P}_y(\mathcal{C}_y(\mathcal{E}_{\tau_1(y)})) &= \mu(\mathcal{E}_{\tau_1(y)}) \\ &\stackrel{(5.22)}{=} \exp\left(-\frac{2\rho\tau_1(y)}{\sqrt{2\pi\mathcal{K}m}}\right), \end{aligned} \quad (5.175)$$

we obtain for the l.h.s. of (5.172) that

$$\begin{aligned} \mathbb{P}_y(dY(\cdot + \tau_1(y))) &\stackrel{(5.173)}{\geq} \mathbb{P}(dY(\cdot + \tau_1(y)) | \mathcal{C}_y(\mathcal{E}_{\tau_1(y)})) \mathbb{P}_y(\mathcal{C}_y(\mathcal{E}_{\tau_1(y)})) \\ &\stackrel{(5.174), (5.175)}{=} \mathbb{P}(dY(\cdot + \tau_1(y)) | Y(\tau_1(y))) \exp\left(-\frac{2\rho\tau_1(y)}{\sqrt{2\pi\mathcal{K}m}}\right) \end{aligned} \quad (5.176)$$

where $Y(\tau_1(y))$ is given by (5.168) with (5.169) and (5.170).

To give a lower bound for the l.h.s. of (5.162), namely for $\mathbb{P}_y(dY)$ with $dY \subset O$, we now define events on which the process starting in $Y(\tau_1) = (L, V_1, \sigma_1)$ with $-C \leq V_1 \leq -B$ reaches a state in the overlap set O defined in (5.159). With that we obtain an estimate for

$$\mathbb{P}(dY | Y(\tau_1)). \quad (5.177)$$

for $dY \subset O$, which gives together with (5.176) a lower bound for (5.162).

Consider τ_1 with

$$0 \leq \tau_1 \leq 2t_B \quad (5.178)$$

and

$$Y(\tau_1) = (L, V_1, \sigma_1) \quad (5.179)$$

with

$$-C \leq V_1 \leq -B. \quad (5.180)$$

Note that these are the conditions on τ_1 and $Y(\tau_1)$ for which (5.176) holds. If $\sigma_1 = 1$, consider the event $\mathcal{E}_{V_1, \tau_1}^i \subset \hat{\Omega}$ with

$$\mathcal{E}_{V_1, \tau_1}^i := \{\text{Exactly one atom enters } \Lambda \text{ during } \tau_1 \text{ and } \tau_2 \text{ with velocity} \quad (5.181)$$

$$v \in V_{V_1}^i := \left(\frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} - \frac{M-m}{2m} |V_1|, \right. \\ \left. \frac{M-3m}{2m} \frac{B}{5} - \frac{M-m}{2m} |V_1| \right) \quad (5.182)$$

such that it collides with the molecule at collision time

$$\tau \in T_{V_1, \tau_1}^i(v) := \left(\frac{4L + |V_1|(\tau_1 - \frac{10L}{B} \frac{M-m}{M-3m}) + \frac{10L}{B} \frac{2m}{M-3m} |v|}{\frac{2m}{M+m} (|V_1| + |v|)}, \right. \\ \left. \frac{4L + |V_1|(\tau_1 - \frac{10L}{B} \frac{M}{M-3m} \frac{M-m}{M+m}) + \frac{10L}{B} \frac{M}{M-3m} \frac{2m}{M+m} |v|}{\frac{2m}{M+m} (|V_1| + |v|)} \right) \quad (5.183)$$

and if $\sigma_1 = -1$ consider the event $\mathcal{E}_{V_1, \tau_1}^{ii} \subset \hat{\Omega}$ with

$$\mathcal{E}_{V_1, \tau_1}^{ii} := \{\text{Exactly one atom enters } \Lambda \text{ during } \tau_1 \text{ and } \tau_2 \text{ with velocity} \quad (5.184)$$

$$v \in V_{V_1}^{ii} := \left(\frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1|, \right. \\ \left. \frac{M-3m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1| \right) \quad (5.185)$$

such that it collides with the molecule at collision time

$$\tau \in T_{V_1, \tau_1}^{ii}(v) := \left(\frac{|V_1|(\tau_1 - \frac{10L}{B} \frac{M-m}{M+m} \frac{M}{M-3m}) + \frac{10L}{B} \frac{2m}{M+m} \frac{M}{M-3m} v}{\frac{2m}{M+m} (|V_1| + v)}, \right. \\ \left. \frac{|V_1|(\tau_1 - \frac{10L}{B} \frac{M-m}{M-3m}) + \frac{10L}{B} \frac{2m}{M-3m} v}{\frac{2m}{M+m} (|V_1| + v)} \right) \quad (5.186)$$

Note that τ_2 is determined by V_1, τ_1, v and τ and since these values are bounded, τ_2 is bounded.

First, we show that $\mathcal{E}_{V_1, \tau_1}^i$ and $\mathcal{E}_{V_1, \tau_1}^{ii}$ are well defined. To be precise, we show more, namely that any collision time $\tau \in T_{V_1, \tau_1}^i(v)$ resp. $T_{V_1, \tau_1}^{ii}(v)$ is possible, given that the atom enters Λ between τ_1 and $\tau_1 + \frac{4L}{|V_1|}$ (which is the time when the molecule would reach the wall at L if it moved freely) with velocity $v \in V_{V_1}^i$ resp. $V_{V_1}^{ii}$. For this proof, we first show from which direction the atom in $\mathcal{E}_{V_1, \tau_1}^i$ resp. $\mathcal{E}_{V_1, \tau_1}^{ii}$ enters the interval (Assertion 5.11 resp. Assertion 5.12). Then, we give bounds for the collision time τ , from which we can make conclusions about the direction the molecule travels right before the collision takes place (Assertion

5.13 resp. Assertion 5.14). Finally, by these assertions we prove that $\mathcal{E}_{V_1, \tau_1}^i$ and $\mathcal{E}_{V_1, \tau_1}^{ii}$ are well defined.

Note that these assertions follow by elementary algebra.

Assertion 5.11. Consider $V_{V_1}^i$ as defined in (5.182), then

$$v \in V_{V_1}^i \Rightarrow v < 0,$$

i.e. on $\mathcal{E}_{V_1, \tau_1}^i$ the atom enters from the right.

Proof of Assertion 5.11. Consider $v \in V_{V_1}^i$. Since then

$$v \stackrel{(5.182)}{<} \frac{M-3m}{2m} \frac{B}{5} - \frac{M-m}{2m} |V_1| \stackrel{(5.180)}{<} \frac{M-3m}{2m} \frac{B}{5} - \frac{M-m}{2m} B < 0,$$

the atom enters from the right. □

Assertion 5.12. Consider $V_{V_1}^{ii}$ as defined in (5.185), then

$$v \in V_{V_1}^{ii} \Rightarrow v > 0,$$

i.e. on $\mathcal{E}_{V_1, \tau_1}^{ii}$ the atom enters from the left.

Proof of Assertion 5.12. Since $M > 3m$ we have for $v \in V_{V_1}^{ii}$ that

$$v \stackrel{(5.185)}{>} \frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1| > 0,$$

i.e. on $\mathcal{E}_{V_1, \tau_1}^{ii}$ the atom enters from the left. □

Assertion 5.13. If $\tau \in T_{V_1, \tau_1}^i(v)$ (cf. (5.183)) with $v \in V_{V_1}^i$ (cf. (5.182)), then

$$\tau_1 + \frac{2L}{|V_1|} < \tau < \tau_1 + \frac{4L}{|V_1|}.$$

Proof of Assertion 5.13. By Assertion 5.11 it follows on $V_{V_1}^i$ that

$$-\frac{M-3m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1| < |v| < -\frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1| \quad (5.187)$$

and we obtain that

$$\begin{aligned} \tau &\stackrel{(5.183)}{>} \frac{4L + |V_1|(\tau_1 - \frac{10L}{B} \frac{M-m}{M-3m}) + \frac{10L}{B} \frac{2m}{M-3m} |v|}{\frac{2m}{M+m} (|V_1| + |v|)} \\ &\stackrel{(5.187)}{>} \frac{4L + |V_1|(\tau_1 - \frac{10L}{B} \frac{M-m}{M-3m}) + \frac{10L}{B} \frac{2m}{M-3m} |v|}{\frac{2m}{M+m} (|V_1| - \frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1|)} \\ &= \frac{4L + |V_1|(\tau_1 - \frac{10L}{B} \frac{M-m}{M-3m}) + \frac{10L}{B} \frac{2m}{M-3m} |v|}{|V_1| - \frac{M-3m}{M+3m} \frac{B}{5}} \\ &\stackrel{M > 3m}{>} \frac{4L}{|V_1|} + \tau_1 - \frac{10L}{B} \frac{M-m}{M-3m} + \frac{10L}{B} \frac{2m}{M-3m} \frac{|v|}{|V_1|} \\ &= \frac{4L}{|V_1|} + \tau_1 - \frac{10L}{B(M-3m)} \left((M-m) - 2m \frac{|v|}{|V_1|} \right) \\ &\stackrel{(5.187)}{>} \frac{4L}{|V_1|} + \tau_1 - \frac{10L}{B(M-3m)} \left((M-m) + \frac{M-3m}{5} \frac{B}{|V_1|} - (M-m) \right) \\ &= \tau_1 + \frac{2L}{|V_1|} \end{aligned}$$

and that

$$\begin{aligned} \tau &\stackrel{(5.183)}{<} \frac{4L + |V_1|(\tau_1 - \frac{10L}{B} \frac{M}{M-3m} \frac{M-m}{M+m}) + \frac{10L}{B} \frac{M}{M-3m} \frac{2m}{M+m} |v|}{\frac{2m}{M+m} (|V_1| + |v|)} \\ &= \frac{4L + |V_1| \tau_1 - \frac{10L}{B} \frac{M}{M-3m} (\frac{M-m}{M+m} |V_1| - \frac{2m}{M+m} |v|)}{\frac{2m}{M+m} (|V_1| + |v|)}. \end{aligned} \quad (5.188)$$

Since

$$\begin{aligned} &\frac{M-m}{M+m} |V_1| - \frac{2m}{M+m} |v| \\ &> \frac{M-m}{M+m} |V_1| - \frac{2m}{M+m} \left(\frac{M-m}{2m} |V_1| - \frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} \right) \\ &= \frac{M-3m}{M+3m} \frac{B}{5} \\ &> 0 \end{aligned}$$

and

$$\frac{10L}{B} \frac{M}{M-3m} \stackrel{M>3m}{>} \frac{8L}{B} \stackrel{(5.171),(5.166)}{\geq} \tau_1 + \frac{4L}{|V_1|}, \quad (5.189)$$

we can estimate

$$\begin{aligned} (5.188) &= \frac{4L + |V_1|\tau_1 - \frac{10L}{B} \frac{M}{M-3m} \left(\frac{M-m}{M+m} |V_1| - \frac{2m}{M+m} |v| \right)}{\frac{2m}{M+m} (|V_1| + |v|)} \\ &\stackrel{(5.189)}{<} \frac{4L + |V_1|\tau_1 - \left(\tau_1 + \frac{4L}{|V_1|} \right) \left(\frac{M-m}{M+m} |V_1| - \frac{2m}{M+m} |v| \right)}{\frac{2m}{M+m} (|V_1| + |v|)} \\ &= \frac{4L + \frac{2m}{M+m} \tau_1 (|V_1| + |v|) - 4L \frac{M-m}{M+m} + \frac{4L}{|V_1|} \frac{2m}{M+m} |v|}{\frac{2m}{M+m} (|V_1| + |v|)} \\ &= \frac{4L \left(1 - \frac{M-m}{M+m} + \frac{1}{|V_1|} \frac{2m}{M+m} |v| \right) + \frac{2m}{M+m} \tau_1 (|V_1| + |v|)}{\frac{2m}{M+m} (|V_1| + |v|)} \\ &= \frac{4L \frac{2m}{M+m} \left(\frac{|V_1| + |v|}{|V_1|} \right) + \frac{2m}{M+m} \tau_1 (|V_1| + |v|)}{\frac{2m}{M+m} (|V_1| + |v|)} \\ &= \tau_1 + \frac{4L}{|V_1|}, \end{aligned}$$

so that

$$\tau < \tau_1 + \frac{4L}{|V_1|}.$$

□

Assertion 5.14. If $\tau \in T_{V_1, \tau_1}^{ii}(v)$ (cf. (5.186)) with $v \in V_{V_1}^{ii}$ (cf. (5.185)), then

$$\tau_1 + \frac{L}{|V_1|} < \tau < \tau_1 + \frac{2L}{|V_1|}.$$

Proof of Assertion 5.14. Consider $\tau \in T_{V_1, \tau_1}^{ii}(v)$, then we have that

$$\begin{aligned} \tau &> \frac{|V_1| \left(\tau_1 - \frac{10L}{B} \frac{M-m}{M+m} \frac{M}{M-3m} \right) + \frac{10L}{B} \frac{2m}{M+m} \frac{M}{M-3m} |v|}{\frac{2m}{M+m} (|V_1| + |v|)} \\ &= \frac{|V_1| \tau_1 + \frac{10L}{B} \frac{M}{M-3m} \left(\frac{2m}{M+m} |v| - \frac{M-m}{M+m} |V_1| \right)}{\frac{2m}{M+m} (|V_1| + |v|)}. \end{aligned} \quad (5.190)$$

Since by Assertion 5.12, on $V_{V_1}^{ii} v > 0$, i.e.

$$\frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1| < |v| < \frac{M-3m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1|, \quad (5.191)$$

it follows for $M > 3m$ that

$$\frac{2m}{M+m} |v| - \frac{M-m}{M+m} |V_1| \stackrel{(5.191)}{>} \frac{M-3m}{M+3m} \frac{B}{5} > 0$$

and since

$$\begin{aligned} \frac{10L}{B} \frac{M}{M-3m} &= \frac{4L(M-3m) + L(M-3m) + 5L(M+3m)}{B(M-3m)} \\ &= \frac{4L}{B} + \frac{L}{B} + \frac{5L}{B} \frac{M+3m}{M-3m} \\ &\stackrel{(5.171), (5.166)}{>} \tau_1 + \frac{L}{|V_1|} + \frac{5L}{B} \frac{M+3m}{M-3m} \end{aligned} \quad (5.192)$$

we can estimate

$$\begin{aligned} (5.190) &= \frac{|V_1| \tau_1 + \frac{10L}{B} \frac{M}{M-3m} \left(\frac{2m}{M+m} |v| - \frac{M-m}{M+m} |V_1| \right)}{\frac{2m}{M+m} (|V_1| + v)} \\ &\stackrel{(5.191), (5.192)}{>} \frac{|V_1| \tau_1 + \left(\tau_1 + \frac{L}{|V_1|} + \frac{5L}{B} \frac{M+3m}{M-3m} \right) \left(\frac{2m}{M+m} |v| - \frac{M-m}{M+m} |V_1| \right)}{\frac{2m}{M+m} (|V_1| + v)} \\ &= \frac{\frac{2m}{M+m} \tau_1 (|V_1| + |v|) + \frac{|v|L}{|V_1|} \frac{2m}{M+m} + \frac{2m}{M+m} L}{\frac{2m}{M+m} (|V_1| + v)} \\ &= \frac{\tau_1 (|V_1| + |v|) + \frac{L}{|V_1|} (|V_1| + |v|)}{|V_1| + |v|} \\ &= \tau_1 + \frac{L}{|V_1|}, \end{aligned}$$

and thus

$$\tau > \tau_1 + \frac{L}{|V_1|}.$$

Furthermore, we have that

$$\begin{aligned} \tau &\stackrel{(5.186)}{<} \frac{|V_1| \left(\tau_1 - \frac{10L}{B} \frac{M-m}{M+m} \frac{M+m}{M-3m} \right) + \frac{10L}{B} \frac{2m}{M+m} \frac{M+m}{M-3m} |v|}{\frac{2m}{M+m} (|V_1| + |v|)} \\ &\stackrel{(5.191)}{<} \frac{|V_1| \left(\tau_1 - \frac{10L}{B} \frac{M-m}{M-3m} \right) + 2L + \frac{10L}{B} \frac{M-m}{M-3m} |V_1|}{\frac{2m}{M+m} (|V_1| + \frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1|)} \end{aligned}$$

$$\begin{aligned}
&= \frac{|V_1|\tau_1 + 2L}{|V_1| + \frac{M-3m}{M+m}\frac{B}{5}} \\
&\stackrel{M > 3m}{<} \tau_1 + \frac{2L}{|V_1|}.
\end{aligned}$$

□

We have shown that on $\mathcal{E}_{V_1, \tau_1}^i$ the atom enters from the right (cf. Assertion 5.11) and collides with the molecule during $(\tau_1 + \frac{2L}{|V_1|}, \tau_1 + \frac{4L}{|V_1|})$ (cf. Assertion 5.13), whereas on $\mathcal{E}_{V_1, \tau_1}^{ii}$ the atom enters from the left (cf. Assertion 5.12) and collides during $(\tau_1 + \frac{L}{|V_1|}, \tau_1 + \frac{2L}{|V_1|})$ with the molecule (cf. Assertion 5.14). Using these results, we can show that an atom which collides with pre collision velocity $v \in V_{V_1}^i$ (cf. (5.182)) resp. $V_{V_1}^{ii}$ (cf. (5.185)) coming from the right resp. from the left with the molecule at any time $\tau \in T_{V_1, \tau_1}^i(v)$ (cf. (5.183)) resp. $T_{V_1, \tau_1}^{ii}(v)$ (cf. (5.186)), has entered the interval between τ_1 and $\tau_1 + \frac{4L}{|V_1|}$, given that $Y(\tau_1) = (L, V_1, \sigma_1)$ with $-C \leq V_1 \leq -B$, and that no other atom enters the interval during τ_1 and $\tau_1 + \frac{4L}{|V_1|}$. Recall that $\tau_1 + \frac{4L}{|V_1|}$ is the time when the molecule would reach the wall at L if it moved freely.

Denote by τ_e the entering time of the atom and recall that τ_1 is the time, when the molecule is at L the first time after $t = 0$, and that τ is the time when the molecule and the atom collide.

Consider $Y(\tau_1)$ as given in (5.179) with (5.180), $v \in V_{V_1}^i$ (i.e. the atom is entering from the right) and $\tau \in T_{V_1, \tau_1}^i(v)$. Since then by Assertion 5.13 the collision takes place after $\tau_1 + \frac{2L}{|V_1|}$, which is the time the molecule was reflected at $-L$, but before $\tau_1 + \frac{4L}{|V_1|}$ (which is the time the molecule would reach L again if it moved freely), the sum of the distance the molecule travels between τ_1 and τ , and of the distance the atom travels between τ_e and τ is $4L$. Hence, τ_e is determined by

$$|V_1|(\tau - \tau_1) + |v|(\tau - \tau_e) = 4L,$$

which gives

$$\tau_e = \frac{|V_1|}{|v|}(\tau - \tau_1) + \tau - \frac{4L}{|v|}. \quad (5.193)$$

We then obtain by Assertion 5.13 that

$$\begin{aligned}
\tau_e &\stackrel{(5.193)}{=} \frac{|V_1|}{|v|}(\tau - \tau_1) + \tau - \frac{4L}{|v|} \\
&> \frac{2L}{|v|} + \tau_1 + \frac{2L}{|V_1|} - \frac{4L}{|v|} \\
&= \tau_1 + \frac{2L}{|V_1|} - \frac{2L}{|v|},
\end{aligned}$$

and since

$$\begin{aligned}
|v| &\stackrel{(5.182)}{>} \frac{M-m}{2m}|V_1| - \frac{M-3m}{2m} \frac{B}{5} \\
&\stackrel{|V_1| > \frac{B}{5}}{>} \frac{M-m}{2m}|V_1| - \frac{M-3m}{2m}|V_1| \\
&= |V_1|
\end{aligned}$$

we have that

$$\tau_e > \tau_1. \quad (5.194)$$

For the upper bound of τ_e we estimate by Assertion 5.13 that

$$\begin{aligned}
\tau_e &\stackrel{(5.193)}{=} \frac{|V_1|}{|v|}(\tau - \tau_1) + \tau - \frac{4L}{|v|} \\
&< \frac{4L}{|v|} + \tau_1 + \frac{4L}{|V_1|} - \frac{4L}{|v|} \\
&= \tau_1 + \frac{4L}{|V_1|}.
\end{aligned} \quad (5.195)$$

Consider now $Y(\tau_1)$ as given in (5.179) with (5.180), $v \in V_{V_1}^{ii}$ (i.e. the atom enters from the left) and $\tau \in T_{V_1, \tau_1}^{ii}(v)$. Since then by Assertion 5.14 the collision takes place after $\tau_1 + \frac{L}{|V_1|}$ and before $\tau_1 + \frac{2L}{|V_1|}$, which is the time the molecule would reach $-L$ if it moved freely, the sum of the distance the molecule travels between τ_1 and τ , and of the distance the atom travels between τ_e and τ is $2L$. Hence, τ_e is determined by

$$|V_1|(\tau - \tau_1) + |v|(\tau_e - \tau) = 2L,$$

which gives

$$\tau_e = \frac{|V_1|}{|v|}(\tau - \tau_1) + \tau - \frac{2L}{|v|}. \quad (5.196)$$

We then obtain by Assertion 5.14 that

$$\begin{aligned}
\tau_e &\stackrel{(5.196)}{=} \frac{|V_1|}{|v|}(\tau - \tau_1) + \tau - \frac{2L}{|v|} \\
&> \frac{L}{|v|} + \tau_1 + \frac{L}{|V_1|} - \frac{2L}{|v|} \\
&= \tau_1 + \frac{L}{|V_1|} - \frac{L}{|v|}
\end{aligned}$$

and since for $v \in V_{V_1}^{ii}$

$$\begin{aligned} |v| &> \frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} + \frac{M-m}{2m} |V_1| \\ &= \frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} + \frac{M-3m}{2m} |V_1| + |V_1| \\ &\stackrel{M>3m}{>} |V_1|, \end{aligned}$$

we have that

$$\tau_e > \tau_1. \quad (5.197)$$

For the upper bound of τ_e we obtain by Assertion 5.14 that

$$\begin{aligned} \tau_e &\stackrel{(5.196)}{=} \frac{|V_1|}{|v|} (\tau - \tau_1) - \tau - \frac{2L}{|v|} \\ &< \frac{2L}{|v|} + \tau_1 + \frac{2L}{|V_1|} - \frac{2L}{|v|} \\ &= \tau_1 + \frac{2L}{|V_1|}. \end{aligned} \quad (5.198)$$

With (5.194) and (5.195) resp. (5.197) and (5.198) we have shown that $\mathcal{E}_{V_1, \tau_1}^i$ and $\mathcal{E}_{V_1, \tau_1}^{ii}$ are well defined and any collision time $\tau \in T_{V_1, \tau_1}^i(v)$ resp. $T_{V_1, \tau_1}^{ii}(v)$ is possible, given that the atom enters Λ between τ_1 and τ_2 .

Before we show that on $\mathcal{E}_{V_1, \tau_1}^i$ and $\mathcal{E}_{V_1, \tau_1}^{ii}$ the process reaches a state in O (cf. (5.159)), we identify the corresponding (v, q) -set of $\mathcal{E}_{V_1, \tau_1}^i$ and $\mathcal{E}_{V_1, \tau_1}^{ii}$, where q is the position of the atom at time $t = 0$.

On $\mathcal{E}_{V_1, \tau_1}^i$ (cf. (5.181)), the atom which collides with the molecule at time τ with velocity v was at time $t = 0$ at position

$$\begin{aligned} q &= -L + |V_1| \left(\tau - \left(\tau_1 + \frac{2L}{|V_1|} \right) \right) + |v|\tau \\ &= -3L + (|V_1| + |v|)\tau - |V_1|\tau_1. \end{aligned} \quad (5.199)$$

With $\tau \in T_{V_1, \tau_1}^i(v)$ (cf. (5.183)) we obtain that the (v, q) -set described in $\mathcal{E}_{V_1, \tau_1}^i$ is

$$\mathcal{VQ}_{V_1, \tau_1}^i := \{(v, q) : v \in V_{V_1}^i, q \in Q_{V_1, \tau_1}^i(v)\} \quad (5.200)$$

with $V_{V_1}^i$ as given in (5.182) and

$$\begin{aligned} Q_{V_1, \tau_1}^i(v) &:= \\ &= \left(-3L + \frac{M+m}{2m}4L + \frac{M-m}{2m}|V_1|\tau_1 - \frac{10L}{B} \frac{M+m}{M-3m} \left(|V_1| \frac{M-m}{2m} - |v| \right), \right. \\ &\quad \left. -3L + \frac{M+m}{2m}4L + \frac{M-m}{2m}|V_1|\tau_1 - \frac{10L}{B} \frac{M}{M-3m} \left(|V_1| \frac{M-m}{2m} - |v| \right) \right). \end{aligned} \quad (5.201)$$

Note that (5.201) follows by plugging in the bounds of $T_{V_1, \tau_1}^i(v)$ (cf. (5.183)) in (5.199). On $\mathcal{E}_{V_1, \tau_1}^{ii}$ (cf. (5.184)), the atom which collides with the molecule at time τ with velocity v was at time $t = 0$ at position

$$\begin{aligned} q &= L - |V_1|(\tau - \tau_1) - |v|\tau \\ &= L - (|V_1| + |v|)\tau + |V_1|\tau_1. \end{aligned} \quad (5.202)$$

With $\tau \in T_{V_1, \tau_1}^{ii}(v)$ (cf. (5.186)), we obtain that the (v, q) -set described in $\mathcal{E}_{V_1, \tau_1}^{ii}$ is given by

$$\mathcal{V}Q_{V_1, \tau_1}^{ii} := \{(v, q) : v \in V_{V_1}^{ii}, q \in Q_{V_1, \tau_1}^{ii}(v)\} \quad (5.203)$$

with $V_{V_1}^{ii}$ given in (5.185) and

$$\begin{aligned} Q_{V_1, \tau_1}^{ii}(v) &:= \left(L - \frac{M-m}{2m}|V_1|\tau_1 - \frac{10L}{B} \frac{M+m}{M-3m} \left(|v| - \frac{M-m}{2m}|V_1| \right), \right. \\ &\quad \left. L - \frac{M-m}{2m}|V_1|\tau_1 - \frac{10L}{B} \frac{M}{M-3m} \left(|v| - \frac{M-m}{2m}|V_1| \right) \right). \end{aligned} \quad (5.204)$$

Note that (5.204) follows by plugging in the bounds of $T_{V_1, \tau_1}^{ii}(v)$ (cf. (5.186)) in (5.202).

Finally, we show if $Y(\tau_1)$ is given by (5.179) with (5.180) and τ_1 as given in (5.178), then on $\mathcal{E}_{V_1, \tau_1}^i$ (cf. (5.181)) resp. $\mathcal{E}_{V_1, \tau_1}^{ii}$ (cf. (5.184)) the molecule is alone in Λ at time τ_2 , and $\tau_2 \in \mathcal{T}_2$ (cf. (5.161)), $V_2 \in \mathcal{V}_2$, (cf. (5.160)), $\sigma_2 = 1$, i.e.

$$Y \in O \text{ (cf. (5.159))}. \quad (5.205)$$

Recall, if $\sigma_1 = 1$, we consider $\mathcal{E}_{V_1, \tau_1}^i$ and if $\sigma_1 = -1$, we consider $\mathcal{E}_{V_1, \tau_1}^{ii}$. Denote by V_{τ_-} the pre collision velocity of the molecule. Note that on $\mathcal{E}_{V_1, \tau_1}^i$

$$V_{\tau_-} = |V_1|, \quad (5.206)$$

since the atom meets the molecule, when the molecule moves in positive direction (cf. Assertion 5.13). On $\mathcal{E}_{V_1, \tau_1}^{ii}$

$$V_{\tau_-} = -|V_1|, \quad (5.207)$$

since the atom meets the molecule, when the molecule moves in negative direction (cf.

Assertion 5.14). The post collision velocity V' of the molecule is then given by

$$V' = \frac{M-m}{M+m}V_{\tau^-} + \frac{2m}{M+m}v \quad (5.208)$$

(cf. (2.1)). Since on $\mathcal{E}_{V_1, \tau_1}^i$

$$V' \stackrel{(5.208), (5.206)}{=} \frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v \quad (5.209)$$

$$\begin{aligned} &\stackrel{(5.182)}{>} \frac{M-m}{M+m}|V_1| + \frac{2m}{M+m} \left(\frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} - \frac{M-m}{2m}|V_1| \right) \\ &= \frac{M-3m}{M+3m} \frac{B}{5} \\ &> 0, \end{aligned} \quad (5.210)$$

and on $\mathcal{E}_{V_1, \tau_1}^{ii}$

$$V' \stackrel{(5.208), (5.207)}{=} -\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v \quad (5.211)$$

$$\begin{aligned} &\stackrel{(5.185)}{>} -\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m} \left(\frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} + \frac{M-m}{2m}|V_1| \right) \\ &= \frac{M-3m}{M+3m} \frac{B}{5} \\ &> 0 \end{aligned} \quad (5.212)$$

and the molecule reaches L without an additional collision on both events, we have that

$$V_2 = -V'. \quad (5.213)$$

Since (5.208) is a linear function of v if V_{τ^-} is given, we obtain on $\mathcal{E}_{V_1, \tau_1}^i$ with $v \in V_{V_1}^i$ (cf. (5.182)) by (5.209) and (5.213) for V_2 any value with

$$\begin{aligned} V_2 &= -\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}v \\ &> -\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m} \left(\frac{M-3m}{2m} \frac{B}{5} - \frac{M-m}{2m}|V_1| \right) \\ &= -\frac{M-3m}{M+m} \frac{B}{5} \end{aligned} \quad (5.214)$$

and

$$\begin{aligned} V_2 &= -\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}v \\ &< -\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m} \left(\frac{M-3m}{M+3m} \frac{M+m}{2m} \frac{B}{5} - \frac{M-m}{2m}|V_1| \right) \end{aligned}$$

$$= -\frac{M - 3m B}{M + 3m \frac{B}{5}}, \quad (5.215)$$

and since on $\mathcal{E}_{V_1, \tau_1}^{ii}$ $v \in V_{V_1}^{ii}$ (cf. (5.185)) we obtain by (5.211) and (5.213) for V_2 any value with

$$\begin{aligned} V_2 &= -\frac{M - m}{M + m}|V_1| - \frac{2m}{M + m}v \\ &> -\frac{M - m}{M + m}|V_1| - \frac{2m}{M + m} \left(\frac{M - 3m B}{2m \frac{B}{5}} - \frac{M - m}{2m}|V_1| \right) \\ &= -\frac{M - 3m B}{M + m \frac{B}{5}} \end{aligned} \quad (5.216)$$

and

$$\begin{aligned} V_2 &= -\frac{M - m}{M + m}|V_1| - \frac{2m}{M + m}v \\ &< -\frac{M - m}{M + m}|V_1| - \frac{2m}{M + m} \left(\frac{M - 3m \frac{M + m B}{2m \frac{B}{5}}}{M + 3m} - \frac{M - m}{2m}|V_1| \right) \\ &= -\frac{M - 3m B}{M + 3m \frac{B}{5}}. \end{aligned} \quad (5.217)$$

Hence, by (5.214), (5.215), (5.216) and (5.217) we have on $\mathcal{E}_{V_1, \tau_1}^i$ and on $\mathcal{E}_{V_1, \tau_1}^{ii}$ that

$$V_2 \in \mathcal{V}_2 \quad (5.218)$$

(cf. (5.160)).

To show (5.205) we also have to specify the possible values of τ_2 on $\mathcal{E}_{V_1, \tau_1}^i$ (cf. (5.181)) and $\mathcal{E}_{V_1, \tau_1}^{ii}$ (cf. (5.184)).

The value of τ_2 on $\mathcal{E}_{V_1, \tau_1}^i$ is given as follows. By Assertion 5.13 the collision takes place after $\tau_1 + \frac{2L}{|V_1|}$, where the molecule was reflected at $-L$, but before $\tau_1 + \frac{4L}{|V_1|}$, where the molecule would reach L again if it moved freely. Hence, after the molecule is reflected at L at time τ_1 , it reaches $-L$ and collides afterwards with the atom. Since $V' > 0$ (cf. (5.210)) the molecule reaches again L . That means that the molecule covers a length of $4L$ during τ_1 and τ_2 . Since it has speed V_1 during τ_1 and τ , and speed V' during τ and τ_2 , we have that

$$|V_1|(\tau - \tau_1) + V'(\tau_2 - \tau) = 4L,$$

which determines τ_2 by

$$\begin{aligned} \tau_2 &= \frac{4L - |V_1|(\tau - \tau_1)}{V'} + \tau \\ &\stackrel{(5.209)}{=} \frac{4L - |V_1|(\tau - \tau_1)}{\frac{M - m}{M + m}|V_1| + \frac{2m}{M + m}v} + \tau \end{aligned}$$

$$= \frac{4L + |V_1|\tau_1 - \frac{2m}{M+m}(|V_1| + |v|)\tau}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|}. \quad (5.219)$$

Plugging in

$$\tau = \frac{q + 3L + |V_1|\tau_1}{|V_1| + |v|}, \quad (5.220)$$

(which we obtain by (5.199)) into (5.219) yields

$$\begin{aligned} \tau_2 &= \frac{4L + |V_1|\tau_1 - \frac{2m}{M+m}(|V_1| + |v|)\tau}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} \\ &\stackrel{(5.220)}{=} \frac{4L + |V_1|\tau_1 - \frac{2m}{M+m}(q + 3L + |V_1|\tau_1)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} \\ &= \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m}(q + 3L)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|}. \end{aligned} \quad (5.221)$$

Since (5.221) is a linear function of q if V_1, τ_1, v are given, we obtain for τ_2 on $\mathcal{E}_{V_1, \tau_1}^i$ all values with

$$\begin{aligned} \tau_2 &\stackrel{(5.221)}{=} \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m}(q + 3L)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} \\ &\stackrel{(5.201)}{>} \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} - \\ &\quad - \frac{\frac{2m}{M+m} \left(\frac{M+m}{2m}4L + \frac{M-m}{2m}|V_1|\tau_1 - \frac{10L}{B} \frac{M}{M-3m} \left(|V_1| \frac{M-m}{2m} - |v| \right) \right)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} \\ &= \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m} \left(\frac{M+m}{2m}4L + \frac{M-m}{2m}|V_1|\tau_1 \right)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} + \frac{10L}{B} \frac{M}{M-3m} \\ &= \frac{10L}{B} \frac{M}{M-3m} \end{aligned} \quad (5.222)$$

and

$$\begin{aligned} \tau_2 &\stackrel{(5.221)}{=} \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m}(q + 3L)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} \\ &\stackrel{(5.201)}{<} \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} - \\ &\quad - \frac{\frac{2m}{M+m} \left(\frac{M+m}{2m}4L + \frac{M-m}{2m}|V_1|\tau_1 - \frac{10L}{B} \frac{M+m}{M-3m} \left(|V_1| \frac{M-m}{2m} - |v| \right) \right)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} \end{aligned}$$

$$\begin{aligned}
&= \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m} \left(\frac{M+m}{2m}4L + \frac{M-m}{2m}|V_1|\tau_1 \right)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} + \frac{10L}{B} \frac{M+m}{M-3m} \\
&= \frac{10L}{B} \frac{M+m}{M-3m}
\end{aligned} \tag{5.223}$$

since $q \in Q_{V_1, \tau_1}^i(v)$ (cf. (5.201)). Note that the bounds (5.222) and (5.223) are independent of v , i.e. for any given v one obtains the same range for the values of τ_2 .

On $\mathcal{E}_{V_1, \tau_1}^{ii}$ τ_2 is determined by the following. By Assertion 5.14 the collision takes place before $\tau_1 + \frac{2L}{|V_1|}$, where the molecule would reach $-L$ if it moved freely. Hence, before the molecule may reach $-L$ after τ_1 , it collides with the atom and since $V' > 0$ (cf. (5.212)) the molecule reaches again L without having been at $-L$. That means that the molecule travels the same distance during τ_1 and τ (with speed $|V_1|$) as during τ and τ_2 (with speed V'), i.e.

$$|V_1|(\tau - \tau_1) = V'(\tau_2 - \tau),$$

which gives

$$\begin{aligned}
\tau_2 &= \frac{|V_1|(\tau - \tau_1)}{V'} + \tau \\
&\stackrel{(5.211)}{=} \frac{|V_1|(\tau - \tau_1)}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v} + \tau \\
&= \frac{\frac{2m}{M+m}(|V_1| + |v|)\tau - |V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v}.
\end{aligned} \tag{5.224}$$

For an equivalent expression for τ , we use equation (5.202), which gives

$$\tau = \frac{-q + L + |V_1|\tau_1}{|V_1| + |v|}. \tag{5.225}$$

Plugging this into (5.224) we obtain that

$$\begin{aligned}
\tau_2 &= \frac{\frac{2m}{M+m}(|V_1| + |v|)\tau - |V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v} \\
&\stackrel{(5.225)}{=} \frac{\frac{2m}{M+m}(-q + L + |V_1|\tau_1) - |V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v} \\
&= \frac{\frac{2m}{M+m}(-q + L) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v}.
\end{aligned} \tag{5.226}$$

Since (5.226) is a linear function of q if V_1, τ_1, v are given, we obtain for τ_2 on $\mathcal{E}_{V_1, \tau_1}^{ii}$ all

values with

$$\begin{aligned}
\tau_2 &\stackrel{(5.226)}{=} \frac{\frac{2m}{M+m}(-q+L) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}|v|} \\
&\stackrel{(5.204)}{>} \frac{\frac{2m}{M+m} \left(- \left(L - \frac{M-m}{2m}|V_1|\tau_1 - \frac{10L}{B} \frac{M}{M-3m} \left(|v| - \frac{M-m}{2m}|V_1| \right) \right) + L \right)}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}|v|} - \\
&\quad - \frac{\frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}|v|} \\
&= \frac{\frac{M-m}{M+m}|V_1|\tau_1 + \frac{10L}{B} \frac{M}{M-3m} \left(\frac{2m}{M+m}|v| - \frac{M-m}{M+m}|V_1| \right) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}|v|} \\
&= \frac{10L}{B} \frac{M}{M-3m} \tag{5.227}
\end{aligned}$$

and

$$\begin{aligned}
\tau_2 &= \frac{\frac{2m}{M+m}(-q+L) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}|v|} \\
&\stackrel{(5.204)}{<} \frac{\frac{2m}{M+m} \left(- \left(L - \frac{M-m}{2m}|V_1|\tau_1 - \frac{10L}{B} \frac{M+m}{M-3m} \left(|v| - \frac{M-m}{2m}|V_1| \right) \right) + L \right)}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}|v|} - \\
&\quad - \frac{\frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}|v|} \\
&= \frac{\frac{M-m}{M+m}|V_1|\tau_1 + \frac{10L}{B} \frac{M+m}{M-3m} \left(\frac{2m}{M+m}(|v| - \frac{M-m}{M+m}|V_1|) \right) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}|v|} \\
&= \frac{10L}{B} \frac{M+m}{M-3m}, \tag{5.228}
\end{aligned}$$

since $q \in Q_{V_1, \tau_1}^{ii}(v)$ (cf. (5.204)). Since the interval with bounds (5.222) and (5.223) resp. (5.227) and (5.228) is \mathcal{T}_2 (cf. (5.161)), it follows that on $\mathcal{E}_{V_1, \tau_1}^i$ and on $\mathcal{E}_{V_1, \tau_1}^{ii}$

$$\tau_2 \in \mathcal{T}_2. \tag{5.229}$$

At last we show that $\sigma_2 = 1$. Recall that the value of σ changes as soon as the molecule is reflected at $-L$ or L , and that $\sigma_1 = \sigma(\tau_1)$.

Recall, that if $\sigma_1 = 1$, we consider $\mathcal{E}_{V_1, \tau_1}^i$ (cf. (5.181)). Then, by Assertion 5.13 the molecule reaches, after it was reflected at L at time τ_1 , the wall at $-L$ and collides then with the atom and $V' > 0$ (cf. (5.210)), i.e. the molecule reaches again L , which gives

$$\sigma_2 = \sigma_1 = 1.$$

If $\sigma_1 = -1$, we consider $\mathcal{E}_{V_1, \tau_1}^{ii}$. Then, by Assertion 5.14, before the molecule may reach $-L$

after τ_1 , it collides with the atom and $V' > 0$ (cf. (5.212)). Hence, the molecule reaches again L without having been at $-L$ after τ_1 , which gives

$$\sigma_2 = -\sigma_1 = 1. \quad (5.230)$$

Altogether, we have shown by (5.218), (5.229) and (5.230) that for $Y(\tau_1)$ given in (5.179) with (5.180) and with τ_1 as given in (5.178) on $\mathcal{E}_{V_1, \tau_1}^i$ (cf. (5.181)) resp. $\mathcal{E}_{V_1, \tau_1}^{ii}$ (cf. (5.184)), the molecule reaches the wall at L the second time at time $\tau_2 \in \mathcal{T}_2$ (cf. (5.161)) with $V_2 \in \mathcal{V}_2$, (cf. (5.160)) and $\sigma_2 = 1$. To obtain (5.205), namely

$$Y \in O,$$

we still have to show that the molecule is alone in Λ at time τ_2 .

On both events, $\mathcal{E}_{V_1, \tau_1}^i$ and $\mathcal{E}_{V_1, \tau_1}^{ii}$, there is exactly one atom which enters Λ between τ_1 and τ_2 . On $\mathcal{E}_{V_1, \tau_1}^i$ this atom enters Λ from the right (cf. Assertion 5.11), i.e. it is to the right of the molecule. Since the molecule is at the right bound of Λ at time τ_2 , the atom must have left the interval before τ_2 . Hence, the molecule is alone at time τ_2 on $\mathcal{E}_{V_1, \tau_1}^i$.

On $\mathcal{E}_{V_1, \tau_1}^{ii}$, the atom is to the left of the molecule, i.e. if the atom leaves the interval, it will leave the interval on the left side, i.e. at $-L$. Note that the atom collides after time $\tau_1 + \frac{L}{|V_1|}$ but before $\tau_1 + \frac{2L}{|V_1|}$ (cf. Assertion 5.14), i.e. the molecule gets hit between $-L$ and 0. By (2.2)

$$v' = -\frac{M-m}{M+m}|v| - \frac{2M}{M+m}|V_1| < 0 \quad (5.231)$$

and we have that $V' > 0$ (cf. (5.212)). Furthermore,

$$|v'| \stackrel{(5.231)}{=} \frac{M-m}{M+m}|v| + \frac{2M}{M+m}|V_1| > |V_1| \stackrel{(5.180)}{>} B \stackrel{(5.218)}{>} |V_2| \stackrel{(5.213)}{=} |V'|,$$

i.e. the atom is faster than the molecule and has to travel a shorter distance to $-L$ than the molecule to L : The atom leaves Λ before the molecule reaches L , i.e. before τ_2 . Since no other atom enters the interval until τ_2 , on $\mathcal{E}_{V_1, \tau_1}^{ii}$ the molecule is alone at time τ_2 .

Until now we have shown that given τ_1 with (5.178) and $Y(\tau_1)$ as given in (5.179) with (5.180), then on $\mathcal{E}_{V_1, \tau_1}^i$ (cf. (5.181)) resp. on $\mathcal{E}_{V_1, \tau_1}^{ii}$ (cf. (5.184))

$$Y \in O \text{ (cf. (5.159))}.$$

The exact value of Y is determined by the velocity v and the position q of the incoming atom at time $t = 0$ by the following function. Note that the latter event is controlled by the Poisson field and that $(v, q) \in \mathcal{VQ}_{V_1, \tau_1}^i$ resp. $\mathcal{VQ}_{V_1, \tau_1}^{ii}$, which is the corresponding (v, q) -set of $\mathcal{E}_{V_1, \tau_1}^i$ resp. $\mathcal{E}_{V_1, \tau_1}^{ii}$, i.e. the set in which the atom in $\mathcal{E}_{V_1, \tau_1}^i$ resp. $\mathcal{E}_{V_1, \tau_1}^{ii}$ must lie at time $t = 0$. Equations (5.209) and (5.221) resp. (5.211) and (5.226) define the following

1-1-map from $\mathcal{VQ}_{V_1, \tau_1}^i$ resp. $\mathcal{VQ}_{V_1, \tau_1}^{ii}$ to the (V_2, τ_2) -set $\mathcal{V}_2 \times \mathcal{T}_2$:

$$\begin{aligned} \Phi_{V_1, \tau_1}^i : \mathcal{VQ}_{V_1, \tau_1}^i &\rightarrow \mathcal{V}_2 \times \mathcal{T}_2 \\ (v, q) &\mapsto (V_2, \tau_2) \\ &\stackrel{(5.209), (5.221)}{=} \left(-\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}v, \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m}(q+3L)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} \right) \end{aligned} \quad (5.232)$$

where $\mathcal{VQ}_{V_1, \tau_1}^i$ is given in (5.200), \mathcal{V}_2 in (5.160), \mathcal{T}_2 in (5.161), and

$$\begin{aligned} \Phi_{V_1, \tau_1}^{ii} : \mathcal{VQ}_{V_1, \tau_1}^{ii} &\rightarrow \mathcal{V}_2 \times \mathcal{T}_2 \\ (v, q) &\mapsto (V_2, \tau_2) \\ &\stackrel{(5.211), (5.226)}{=} \left(\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}v, \frac{\frac{2m}{M+m}(-q+L) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v} \right) \end{aligned} \quad (5.233)$$

where $\mathcal{VQ}_{V_1, \tau_1}^{ii}$ is given in (5.203).

Assertion 5.15. Φ_{V_1, τ_1}^i (cf. (5.232)) and Φ_{V_1, τ_1}^{ii} (cf. (5.233)) are bijections.

Proof of Assertion 5.15. To show that Φ_{V_1, τ_1}^i resp. Φ_{V_1, τ_1}^{ii} maps

$$\mathcal{VQ}_{V_1, \tau_1}^i = \{(v, q) : v \in V_{V_1}^i, q \in D_q^i(v)\}$$

(cf. (5.200)) resp.

$$\mathcal{VQ}_{V_1, \tau_1}^{ii} = \{(v, q) : v \in V_{V_1}^{ii}, q \in D_q^{ii}(v)\}$$

(cf. (5.203)) bijectively to

$$\begin{aligned} \mathcal{V}_2 \times \mathcal{T}_2 &= \\ &\stackrel{(5.160), (5.161)}{=} \left(-\frac{M-3m}{M+m} \frac{B}{5}, -\frac{M-3m}{M+3m} \frac{B}{5} \right) \times \left(\frac{10L}{B} \frac{M}{M-3m}, \frac{10L}{B} \frac{M+m}{M-3m} \right), \end{aligned}$$

we first show the surjectivity of Φ_{V_1, τ_1}^i resp. Φ_{V_1, τ_1}^{ii} .

In (5.218) we have shown that on $\mathcal{E}_{V_1, \tau_1}^i$ (cf. (5.181)) resp. on $\mathcal{E}_{V_1, \tau_1}^{ii}$ (cf. (5.184)) V_2 may take any value of \mathcal{V}_2 and no other. Since $V_{V_1}^i$ (cf. (5.182)) resp. $V_{V_1}^{ii}$ (cf. (5.185)) is the corresponding set of $\mathcal{E}_{V_1, \tau_1}^i$ resp. $\mathcal{E}_{V_1, \tau_1}^{ii}$ in respect to v and since the first components of Φ_{V_1, τ_1}^i and Φ_{V_1, τ_1}^{ii} map $v \in V_{V_1}^i$ resp. $v \in V_{V_1}^{ii}$ to V_2 , it follows by (5.218), that the target set of the first component of Φ_{V_1, τ_1}^i resp. Φ_{V_1, τ_1}^{ii} is \mathcal{V}_2 .

In (5.229) we have shown that on $\mathcal{E}_{V_1, \tau_1}^i$ resp. on $\mathcal{E}_{V_1, \tau_1}^{ii}$ τ_2 may take any value in \mathcal{T}_2 and no other. Recall that $\mathcal{VQ}_{V_1, \tau_1}^i$ resp. $\mathcal{VQ}_{V_1, \tau_1}^{ii}$ is the set of (v, q) which corresponds to $\mathcal{E}_{V_1, \tau_1}^i$

resp. $\mathcal{E}_{V_1, \tau_1}^{ii}$. Since the second component of Φ_{V_1, τ_1}^i resp. Φ_{V_1, τ_1}^{ii} maps $(v, q) \in \mathcal{V}_{V_1, \tau_1}^i$ resp. $(v, q) \in \mathcal{V}_{V_1, \tau_1}^{ii}$ to τ_2 , we obtain by (5.229) that the target set of the second component of Φ_{V_1, τ_1}^i resp. Φ_{V_1, τ_1}^{ii} is \mathcal{T}_2 . All in all it follows that Φ_{V_1, τ_1}^i and Φ_{V_1, τ_1}^{ii} are surjective functions. Now we show injectivity of Φ_{V_1, τ_1}^i , i.e.

$$\Phi_{V_1, \tau_1}^i(v, q) = \Phi_{V_1, \tau_1}^i(v', q') \Rightarrow (v, q) = (v', q'). \quad (5.234)$$

Let

$$\Phi_{V_1, \tau_1}^i(v, q) = \Phi_{V_1, \tau_1}^i(v', q').$$

Then,

$$-\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}v = -\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}v' \quad (5.235)$$

and

$$\frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m}(q+3L)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} = \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m}(q'+3L)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v'|}. \quad (5.236)$$

From (5.235) we obtain immediately that $v = v'$. Plugging this into (5.236) yields to

$$\frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m}(q+3L)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|} = \frac{4L + \frac{M-m}{M+m}|V_1|\tau_1 - \frac{2m}{M+m}(q'+3L)}{\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}|v|}$$

Since this is only valid for $q = q'$, the r.h.s. of (5.234) follows.

To show injectivity of Φ_{V_1, τ_1}^{ii} we proceed analogously to the previous case. Let

$$\Phi_{V_1, \tau_1}^{ii}(v, q) = \Phi_{V_1, \tau_1}^{ii}(v', q'),$$

then

$$\frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}v = \frac{M-m}{M+m}|V_1| - \frac{2m}{M+m}v' \quad (5.237)$$

and

$$\frac{\frac{2m}{M+m}(-q+L) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v} = \frac{\frac{2m}{M+m}(-q'+L) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v'}. \quad (5.238)$$

From (5.237) it follows that $v = v'$. Plugging this into (5.238) yields to

$$\frac{\frac{2m}{M+m}(-q+L) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v} = \frac{\frac{2m}{M+m}(-q'+L) - \frac{M-m}{M+m}|V_1|\tau_1}{-\frac{M-m}{M+m}|V_1| + \frac{2m}{M+m}v},$$

which gives $q = q'$, and the r.h.s. of (5.234) follows.

Altogether, it follows that Φ_{V_1, τ_1}^i (cf. (5.232)) and Φ_{V_1, τ_1}^{ii} (cf. (5.233)) map $\mathcal{V}\mathcal{Q}_{V_1, \tau_1}^i$ resp. $\mathcal{V}\mathcal{Q}_{V_1, \tau_1}^{ii}$ bijectively onto the (V_2, τ_2) -set $\mathcal{V}_2 \times \mathcal{T}_2$. □

Finally, using the results of above, we can estimate (5.177), i.e.

$$\mathbb{P}(dY | Y(\tau_1)) \tag{5.239}$$

for $dY \subset O$, $Y(\tau_1)$ as given in (5.179) with (5.180) and τ_1 as given in (5.178), since we have shown that for any $Y(\tau_1)$ as given in (5.179) with (5.180), τ_1 as given in (5.178) and any $dY \subset O$ there are events where exactly one atom with a certain velocity v starts at time $t = 0$ at q and causes “the right” molecular post velocity as well as “the right” τ_2 and σ_2 .

Since different events are necessary for different values of σ_1 such that $Y \in O$, namely $\mathcal{E}_{V_1, \tau_1}^i$ (cf. (5.181)) for $\sigma_1 = 1$ and $\mathcal{E}_{V_1, \tau_1}^{ii}$ (cf. (5.184)) for $\sigma_1 = -1$, we have to distinguish if $\sigma_1 = 1$ or $\sigma_1 = -1$ when estimating (5.239). Thereby, we make use of the distribution of (v, q) (cf. (2.9)) and the transformation of (v, q) to (V_2, τ_2) given by Φ_{V_1, τ_1}^i (cf. (5.232)) resp. Φ_{V_1, τ_1}^{ii} (cf. (5.233)).

Consider τ_1 as given in (5.178) and $Y(\tau_1)$ as given in (5.179) with (5.180). Consider $\sigma_1 = 1$ and $dY \subset O$ with $dY = (dV_2, d\tau_2, \sigma_2 = 1)$.¹ Denote by $\mathcal{C}_{Y(\tau_1)}(\mathcal{E}_{V_1, \tau_1}^i)$ the set of paths for which $Y(\tau_1)$ is as given in (5.178) with $\sigma_1 = 1$ and with τ_1 as given in (5.178) and $\mathcal{E}_{V_1, \tau_1}^i$ occurs. Then, we have that

$$\mathbb{P}(dY | Y(\tau_1)) \geq \mathbb{P}(dY \cap \mathcal{C}_{Y(\tau_1)}(\mathcal{E}_{V_1, \tau_1}^i) | Y(\tau_1)). \tag{5.240}$$

By the results from above, if $Y(\tau_1)$ is as given in (5.179) with (5.180), $\sigma_1 = 1$ and there is one atom (and no other) with $(v, q) \in \Phi_{V_1, \tau_1}^{i-1}(dV_2, d\tau_2)$, then $dY = (dV_2, d\tau_2, \sigma_2 = 1)$. To estimate the r.h.s. of (5.240), denote by $X_{V_1, \tau_1}^{\tau_2}$ the (v, q) -set, such that the atom with velocity v and position q (at time $t = 0$) enters Λ between τ_1 and τ_2 , i.e.

$$X_{V_1, \tau_1}^{\tau_2} = \{(v, q) : v > 0 \wedge q \in (-L - v\tau_2, -L - v\tau_1) \text{ or} \\ v < 0 \wedge q \in (L + |v|\tau_1, L + |v|\tau_2)\}.$$

We then obtain for the r.h.s. of (5.240) that

$$\begin{aligned} & \mathbb{P}(dY \cap \mathcal{C}_{Y(\tau_1)}(\mathcal{E}_{V_1, \tau_1}^i) | Y(\tau_1)) \geq \\ & \geq \mu(\{\mathcal{N}_{\Phi_{V_1, \tau_1}^{i-1}(dV_2, d\tau_2)} = 1\}) \mu(\{\mathcal{N}_{X_{V_1, \tau_1}^{\tau_2} \setminus \Phi_{V_1, \tau_1}^{i-1}(dV_2, d\tau_2)} = 0\}). \end{aligned} \tag{5.241}$$

¹Note that the notation “ $dY = (dV_2, d\tau_2, \sigma_2 = 1)$ ” is of course an abuse of notation, since σ is a discrete variable. We could easily make this by introducing a delta function for σ , but for ease of notation we will not detail that and keep the notation, which will be however not harmful.

Since on O

$$\tau_2 < \frac{10L}{B} \frac{M+m}{M-3m} =: \bar{\tau}, \quad (5.242)$$

it follows that

$$X_{V_1, \tau_1}^{\tau_2} \subset X_{V_1, \tau_1}^{\bar{\tau}}$$

for any $\tau_2 \in \mathcal{T}_2$. Since the entrance times are exponentially distributed, we obtain that

$$\begin{aligned} (5.241) &\geq \mu(\{\mathcal{N}_{\Phi_{V_1, \tau_1}^{i-1}}(dV_2, d\tau_2) = 1\})\mu(\{\mathcal{N}_{X_{V_1, \tau_1}^{\bar{\tau}}} = 0\}) \\ &\stackrel{(2.4), (5.22)}{=} \rho f(\Phi_{V_1, \tau_1}^{i, 1-1}(V_2)) |\det J_{\Phi_{V_1, \tau_1}^{i-1}(V_2, \tau_2)}| \exp\left(-\frac{2(\bar{\tau} - \tau_1)\rho}{\sqrt{2\pi\mathcal{K}m}}\right) dV_2 d\tau_2 \end{aligned} \quad (5.243)$$

where f is the Maxwellian (cf. (2.5)), Φ_{V_1, τ_1}^{i-1} is given by

$$\begin{aligned} \Phi_{V_1, \tau_1}^{i-1} &= (\Phi_{V_1, \tau_1}^{i, 1-1}, \Phi_{V_1, \tau_1}^{i, 2-1}) : \mathcal{V}_2 \times \mathcal{T}_2 \rightarrow \mathcal{V}\mathcal{Q}_{V_1, \tau_1}^i \\ (V_2, \tau_2) &\mapsto (v, q) \\ &= \left(-\frac{M-m}{2m}|V_1| - \frac{M+m}{2m}V_2, \frac{M+m}{2m}V_2\tau_2 + \frac{M+m}{2m}4L + \frac{M-m}{2m}|V_1|\tau_1 - 3L\right) \end{aligned} \quad (5.244)$$

with Jacobian

$$|\det J_{\Phi_{V_1, \tau_1}^{i-1}(V_2, \tau_2)}| = \left(\frac{M+m}{2m}\right)^2 |V_2|. \quad (5.245)$$

Before we continue estimating (5.243), we estimate (5.239) also for $\sigma_1 = -1$.

Denote by $\mathcal{C}_{Y(\tau_1)}(\mathcal{E}_{V_1, \tau_1}^{ii})$ the set of paths corresponding to $\mathcal{E}_{V_1, \tau_1}^{ii}$ (cf. (5.184)) with $Y(\tau_1)$ as given in (5.178) with $\sigma_1 = -1$. By transforming (v, q) to (V_2, τ_2) by Φ_{V_1, τ_1}^{ii} , we obtain for $dY \subset O$ with $dY = (dV_2, d\tau_2, \sigma_2 = 1)$ that

$$\begin{aligned} &\mathbb{P}(dY | Y(\tau_1)) \\ &\geq \mathbb{P}(dY \cap \mathcal{C}_{Y(\tau_1)}(\mathcal{E}_{V_1, \tau_1}^{ii}) | Y(\tau_1)) \\ &= \mu(\{\mathcal{N}_{\Phi_{V_1, \tau_1}^{ii-1}}(dV_2, d\tau_2) = 1\})\mu(\{\mathcal{N}_{X_{V_1, \tau_1}^{\tau_2} \setminus \Phi_{V_1, \tau_1}^{ii-1}}(dV_2, d\tau_2) = 0\}) \\ &\geq \mu(\{\mathcal{N}_{\Phi_{V_1, \tau_1}^{ii-1}}(dV_2, d\tau_2) = 1\})\mu(\{\mathcal{N}_{X_{V_1, \tau_1}^{\bar{\tau}}} = 0\}) \\ &= \rho f(\Phi_{V_1, \tau_1}^{ii, 1-1}(V_2)) |\det J_{\Phi_{V_1, \tau_1}^{ii-1}(V_2, \tau_2)}| \exp\left(-\frac{2(\bar{\tau} - \tau_1)\rho}{\sqrt{2\pi\mathcal{K}m}}\right) dV_2 d\tau_2 \end{aligned} \quad (5.246)$$

with inverse

$$\begin{aligned} \Phi_{V_1, \tau_1}^{ii^{-1}} &= (\Phi_{V_1, \tau_1}^{i,1^{-1}}, \Phi_{V_1, \tau_1}^{i,2^{-1}}) : \mathcal{V}_2 \times \mathcal{T}_2 \rightarrow \mathcal{V}\mathcal{Q}_{V_1, \tau_1}^{ii} \\ (V_2, \tau_2) &\mapsto (v, q) \\ &= \left(\frac{M-m}{2m} |V_1| - \frac{M+m}{2m} V_2, \frac{M+m}{2m} V_2 \tau_2 + L - \frac{M-m}{2m} |V_1| \tau_1 \right), \end{aligned} \quad (5.247)$$

and Jacobian

$$|\det J_{\Phi_{V_1, \tau_1}^{ii^{-1}}(V_2, \tau_2)}| = \left(\frac{M+m}{2m} \right)^2 |V_2|. \quad (5.248)$$

Altogether we obtain by (5.172), (5.175), (5.176), (5.241), (5.243) and (5.246) that for $y \in G_{B,C;0}$ and $dY = (dV_2, d\tau_2, \sigma_2) \subset O$ either

$$\begin{aligned} \mathbb{P}_y(dY) &= \mathbb{P}_y(dV_2, d\tau_2, \sigma_2) \\ &\stackrel{(5.176)}{\geq} \mathbb{P}(dV_2, d\tau_2, \sigma_2 | Y(\tau_1(y))) \exp\left(-\frac{2\rho\tau_1(y)}{\sqrt{2\pi\mathcal{K}m}}\right) \\ &\stackrel{(5.243)}{=} h_{V_1, \tau_1(y)}^i(V_2, \tau_2) dV_2 d\tau_2 \end{aligned}$$

with

$$h_{V_1, \tau_1(y)}^i(V_2, \tau_2) := \rho f(\Phi_{V_1, \tau_1(y)}^{i,1^{-1}}(V_2)) |\det J_{\Phi_{V_1, \tau_1(y)}^{i,1^{-1}}(V_2, \tau_2)}| \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \quad (5.249)$$

or

$$\begin{aligned} \mathbb{P}_y(dY) &= \mathbb{P}_y(dV_2, d\tau_2, \sigma_2) \\ &\stackrel{(5.176)}{\geq} \mathbb{P}(dV_2, d\tau_2, \sigma_2 | Y(\tau_1(y))) \exp\left(-\frac{2\rho\tau_1(y)}{\sqrt{2\pi\mathcal{K}m}}\right) \\ &\stackrel{(5.246)}{=} h_{V_1, \tau_1(y)}^{ii}(V_2, \tau_2) dV_2 d\tau_2 \end{aligned}$$

with

$$\begin{aligned} h_{V_1, \tau_1(y)}^{ii}(V_2, \tau_2) &:= \\ &= \rho f(\Phi_{V_1, \tau_1(y)}^{ii,1^{-1}}(V_2)) |\det J_{\Phi_{V_1, \tau_1(y)}^{ii,1^{-1}}(V_2, \tau_2)}| \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right). \end{aligned} \quad (5.250)$$

Since ρ , the Maxwellian f (cf. (2.5)) and the exponential function are positive functions and

$$|\det J_{\Phi_{V_1, \tau_1(y)}^{i,1^{-1}}(V_2, \tau_2)}| = |\det J_{\Phi_{V_1, \tau_1(y)}^{ii,1^{-1}}(V_2, \tau_2)}|$$

$$\begin{aligned}
& \stackrel{(5.245),(5.248)}{=} \left(\frac{M+m}{2m} \right)^2 |V_2| \\
& \stackrel{V_2 \in \mathcal{V}_2}{>} \left(\frac{M+m}{2m} \right)^2 \frac{M-3m}{M+3m} \frac{B}{5} \\
& \stackrel{M > 3m}{>} 0,
\end{aligned} \tag{5.251}$$

it follows that

$$h_{V_1, \tau_1(y)}^i(V_2, \tau_2) > 0$$

and

$$h_{V_1, \tau_1(y)}^{ii}(V_2, \tau_2) > 0,$$

for any $(V_2, \tau_2) \in \mathcal{V}_2 \times \mathcal{T}_2$ (cf. (5.160), (5.161)) and any $\tau_1(y), V_1$ as defined in (5.165) resp. (5.171). This gives (5.162) of Lemma 5.7

To prove (5.163) of Lemma 5.7, we give a uniform positive lower bound for $h_{V_1, \tau_1(y)}^i$ (cf. (5.249)) and $h_{V_1, \tau_1(y)}^{ii}$ (cf. (5.250)). In the following we write τ_1 instead of $\tau_1(y)$. For given V_1, τ_1 we have for (5.249) that

$$\begin{aligned}
h_{V_1, \tau_1}^i(V_2, \tau_2) &= \rho f(\Phi^{i,1-1}_{V_1, \tau_1}(V_2)) \left(\frac{M+m}{2m} \right)^2 |V_2| \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \\
& \stackrel{(2.4),(5.244)}{=} \rho f\left(-\frac{M-m}{2m}|V_1| - \frac{M+m}{2m}V_2\right) \left(\frac{M+m}{2m} \right)^2 |V_2| \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \\
& \stackrel{(2.5), V_2 < 0}{=} \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\mathcal{K}m}{2}\left(-\frac{M-m}{2m}|V_1| + \frac{M+m}{2m}|V_2|\right)^2} \left(\frac{M+m}{2m} \right)^2 |V_2| \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \\
&= \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\mathcal{K}m}{2}\left(\frac{M-m}{2m}|V_1| - \frac{M+m}{2m}|V_2|\right)^2} \left(\frac{M+m}{2m} \right)^2 |V_2| \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \\
&> \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\mathcal{K}m}{2}\left(\frac{M-m}{2m}|V_1| + \frac{M+m}{2m}|V_2|\right)^2} \left(\frac{M+m}{2m} \right)^2 |V_2| \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \\
& \stackrel{(5.247)}{=} \rho f(\Phi^{ii,1-1}_{V_1, \tau_1}(V_2)) \left(\frac{M+m}{2m} \right)^2 |V_2| \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \\
& \stackrel{(5.250)}{=} h_{V_1, \tau_1}^{ii}(V_2, \tau_2).
\end{aligned} \tag{5.252}$$

Note that equation (5.252) follows since

$$0 < \frac{M-m}{2m}|V_1| - \frac{M+m}{2m}|V_2| < \frac{M-m}{2m}|V_1| + \frac{M+m}{2m}|V_2|.$$

Since for V_1, τ_1 as defined in (5.171) resp. (5.166), and $(V_2, \tau_2) \in \mathcal{V}_2 \times \mathcal{T}_2$ (cf. (5.160),

(5.161))

$$\begin{aligned}
& h_{V_1, \tau_1}^{ii}(V_2, \tau_2) \stackrel{(5.250)}{=} \rho f(\Phi^{ii, 1-1}_{V_1, \tau_1}(V_2)) \left(\frac{M+m}{2m}\right)^2 |V_2| \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \\
& \stackrel{(2.4)}{=} \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\mathcal{K}m}{2}\left(\frac{M-m}{2m}|V_1| + \frac{M+m}{2m}|V_2|\right)^2} \left(\frac{M+m}{2m}\right)^2 |V_2| e^{-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}} \\
& \stackrel{(5.251)}{\geq} \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\mathcal{K}m}{2}\left(\frac{M-m}{2m}C + \frac{M-3m}{2m}\frac{B}{5}\right)^2} \left(\frac{M+m}{2m}\right)^2 \frac{M-3m}{M+3m} \frac{B}{5} e^{-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}},
\end{aligned}$$

we obtain (5.163) by choosing

$$g = \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\mathcal{K}m}{2}\left(\frac{M-m}{2m}C + \frac{M-3m}{2m}\frac{B}{5}\right)^2} \left(\frac{M+m}{2m}\right)^2 \frac{M-3m}{M+3m} \frac{B}{5} e^{-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}} \quad (5.253)$$

with \mathcal{K} given in (2.5), C given in (5.11) and $\bar{\tau}$ given in (5.242). Note that $\bar{\tau}$ depends on L . \square

In Lemma 5.7 we proved the existence of an overlap set for $M > 3m$. To understand which facts cause the necessity to distinguish the different cases $M > 3m$, $M = 3m$, $3m > M > 2m$ and $2m \geq M > m$ when establishing overlap, it may be useful to see how one proceed when identifying an overlap set. Note that we will give a rather rough overview and don't go into detail.

For all states starting in $G_{B,C;0}$ an overlap shall be established. The simplest way to define an overlap set may be such that the molecule is alone in Λ . Then, the overlap set may be defined by a certain interval of molecular velocity and an interval of time, where the molecule is at L the second time after $t = 0$, and $\sigma_2 = 1$, which is the value of σ when the molecule is the second time at L . We follow that and for simplicity we define the overlap set such, that any starting state can reach any state in the overlap set by exactly one collision with an atom.

To control the molecule such that it is at a certain time at a certain position, we have to know the position of the molecule at some time before. Therefore, we introduce τ_1, τ_2 , the time when the molecule is the first resp. the second time after $t = 0$ at L . To control the value of σ_2 , we treat states with different values of $\sigma_1 = \sigma(\tau_1)$ differently: If $\sigma_1 = 1$, we send in an atom between τ_1 and τ_2 such that the molecule is reflected at $-L$ exactly one time between τ_1 and τ_2 , which gives $\sigma_2 = \sigma_1 = 1$ (Scenario I). If $\sigma_1 = -1$, we send in an atom between τ_1 and τ_2 such that the molecule does not touch the wall at $-L$ between τ_1 and τ_2 . This gives $\sigma_2 = -\sigma_1 = 1$ (Scenario II).

Now, one has to identify an interval of molecular velocity V_2 and an interval of arrival time τ_2 , which can be reached by any $y \in G_{B,C;0}$. Doing so, one has to take care of "virtual collisions". This is the case if the molecular post collision velocity V_2 is such that the atom, which causes this velocity, enters Λ after τ_1 (in any scenario). Let τ be the time of collision.

If in Scenario I

$$\tau_1 + \frac{L}{|V_1|} < \tau < \tau_1 + \frac{2L}{|V_1|}, \quad (5.254)$$

then

$$|V_1|(\tau - \tau_1) + |v|(\tau - \tau_1) > 2L \quad (5.255)$$

expresses that the atom enters after τ_1 , whereas if

$$\tau_1 + \frac{2L}{|V_1|} < \tau < \tau_1 + \frac{4L}{|V_1|} \quad (5.256)$$

it has to be satisfied that

$$|V_1|(\tau - \tau_1) + |v|(\tau - \tau_1) > 4L. \quad (5.257)$$

If in Scenario II

$$\tau_1 + \frac{L}{|V_1|} < \tau < \tau_1 + \frac{2L}{|V_1|}, \quad (5.258)$$

and

$$|V_1|(\tau - \tau_1) + |v|(\tau - \tau_1) > 2L, \quad (5.259)$$

then the incoming atom enters after τ_1 . Hence, to exclude virtual collisions either the interval of V_2 has to be such that the corresponding atom is fast enough, namely $|v| > |V_1|$, or the collision time in (5.254), (5.256) and (5.258) has to be restricted. If the overlap set is such, that $|V_2| > |V_1|$, the atom which is send in must have speed $|v| > |V_1|$, i.e. condition (5.255), (5.257) and (5.259) would be satisfied, but the atom may be still in Λ at time τ_2 . Therefore, we choose $|V_2| < B$ (such that the molecule has to be slowed down for any $B < |V_1| < C$), because it can be shown that in this case the atom which is send in has left the interval until τ_2 . Note that then the collision time τ in Scenario I has to satisfy (5.256) to get an overlap respectively to the arrival time τ_2 .

The interval of V_2 , where (5.257) and (5.259) are satisfied and $|V_2| < B$, can be chosen as follows. Using (2.1), in Scenario I we have that

$$|v| = \frac{M - m}{2m}|V_1| - \frac{M + m}{2m}|V_2|.$$

Plugging this into (5.257) gives

$$\left(|V_1| + \frac{M - m}{2m}|V_1| - \frac{M + m}{2m}|V_2| \right) (\tau - \tau_1) > 4L$$

$$\Leftrightarrow \frac{M+m}{2m} (|V_1| - |V_2|) (\tau - \tau_1) > 4L. \quad (5.260)$$

With (5.256) we obtain that (5.260) holds for any τ if

$$\begin{aligned} & \frac{M+m}{2m} (|V_1| - |V_2|) \frac{2L}{|V_1|} > 4L \\ \Leftrightarrow & |V_2| < \frac{M-3m}{M+m} |V_1|. \end{aligned} \quad (5.261)$$

In Scenario II we have with (2.1) that

$$|v| = \frac{M-m}{2m} |V_1| + \frac{M+m}{2m} |V_2|.$$

We obtain by plugging this into (5.259) that

$$\begin{aligned} & \left(|V_1| + \frac{M-m}{2m} |V_1| + \frac{M+m}{2m} |V_2| \right) (\tau - \tau_1) > 2L \\ \Leftrightarrow & \frac{M+m}{2m} (|V_1| + |V_2|) (\tau - \tau_1) > 2L. \end{aligned} \quad (5.262)$$

If (5.258) we have that (5.262) holds for any τ if

$$\begin{aligned} & \frac{M+m}{2m} (|V_1| + |V_2|) \frac{L}{|V_1|} > 2L \\ \Leftrightarrow & |V_2| > -\frac{M-3m}{M+m} |V_1|. \end{aligned} \quad (5.263)$$

If $M > 3m$ and if the interval of V_2 is chosen such that

$$|V_2| < \frac{M-3m}{M+m} B, \quad (5.264)$$

in both scenarios the virtual collisions are excluded, since (5.261) and (5.263) are satisfied and with that (5.257) and (5.259). Since for some $V_2 \in (-\frac{M-3m}{M+m} B, 0)$ there are (V_1, τ_1, σ_1) such that the intervals of arrival times τ_2 are disjoint, the interval of molecular velocity for V_2 has to be restricted in an appropriate manner to obtain overlap. Since $M > 3m$ is the simplest case, Lemma 5.7 is formulated and proved for this case.

If $M \leq 3m$ there are no values for V_2 such that inequality (5.261) is satisfied. Heuristically this is because if $M \leq 3m$ and the values for τ as given in (5.256) aren't restricted, some of the corresponding atoms need to be in Λ before τ_1 to reach the molecule in time, i.e. the collision with these atoms are virtual collisions. Note, the heavier the molecule, the faster the atom has to be to cause the same V_2 . The faster the atom is, the longer is the distance the atom travels until the collision at time τ . It turns out that $3m$ is the lower bound for M such that any atom which collides at time τ as given in (5.256) resp. (5.258) and

causes V_2 as given in (5.264) enters the interval after τ_1 , i.e. there are no virtual collisions. Therefore, if $M \leq 3m$, the interval of τ in Scenario I (cf. (5.256)) has to be restricted, which gives a weaker requirement as (5.261) and one finds values for V_2 where no virtual collisions occur. But if $m < M \leq 2m$, reducing the values of the collision time τ leads to disjoint intervals of arrival times τ_2 for some (V_1, τ_1, σ_1) , i.e. one cannot find a set of a common arrival time and V_2 , which can be reached by every initial condition (V_1, τ_1, σ_1) , given that one atom enters the interval between τ_1 and τ_2 . Therefore, we distinguish if $2m < M \leq 3m$ or $m < M \leq 2m$.

Case $2m < M \leq 3m$

As stated before, in this case in Scenario I the interval of τ (5.256) has to be restricted, such that there are values for V_2 where no virtual collisions occur. It turns out that

$$O = \{\text{Molecule is alone at time } \tau_2, \quad (5.265)$$

$$V_2 \in \mathcal{V}_2 = \left(-\frac{3m - M}{M + m} \frac{B}{2}, -\frac{M}{2(M - m)} \frac{3m - M}{M + m} \frac{B}{2} \right), \quad (5.266)$$

$$\tau_2 \in \mathcal{T}_2 = \left[\frac{4L}{B} + \frac{8L}{B} \frac{2m}{M} \frac{M - m}{3m - M}, \frac{4L}{B} + \frac{8L}{B} \frac{M - m}{3m - M} \right], \quad (5.267)$$

$$\sigma_2 = 1 \}$$

is an overlap set for $2m < M \leq 3m$ and Lemma 5.7 can be proven with

$$\bar{\tau} = \frac{4L}{B} + \frac{8L}{B} \frac{M - m}{3m - M} \quad (5.268)$$

and

$$g = \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\mathcal{K}m}{2} \left(\frac{M-m}{2m} C + \frac{3m-M}{2m} \frac{B}{2} \right)^2} \left(\frac{M+m}{2m} \right)^2 \frac{M}{2(M-m)} \frac{3m-M}{M+m} \frac{B}{2} e^{-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}}. \quad (5.269)$$

Note that then also the values for τ in Scenario II (cf. (5.258)) has to be restricted for any $|V_1|$, since then

$$|V_2| < \frac{3m - M}{M + m} B < \frac{3m - M}{M + m} |V_1|$$

and (5.263) isn't satisfied.

If $M = 3m$ only the collision times in Scenario I has to be restricted and Lemma 5.7 can be shown with redefined

$$O = \{\text{Molecule is alone at time } \tau_2, \quad (5.270)$$

$$V_2 \in \mathcal{V}_2 = \left(-\frac{B}{8}, -\frac{B}{10} \right), \quad (5.271)$$

$$\begin{aligned} \tau_2 \in \mathcal{T}_2 &= \left[\frac{15L}{B}, \frac{16L}{B} \right], \\ \sigma_2 &= 1 \} \end{aligned} \quad (5.272)$$

with

$$\bar{\tau} = \frac{16L}{B} \quad (5.273)$$

and

$$g = \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\mathcal{K}m}{2} \left(\frac{M-m}{2m} C + \frac{M+m}{2m} \frac{B}{8} \right)^2} \left(\frac{M+m}{2m} \right)^2 \frac{B}{10} e^{-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}}. \quad (5.274)$$

Case $m < M \leq 2m$

For $m < M \leq 2m$, in both scenarios the collision time τ in (5.256) and (5.258) has to be restricted: Since in Scenario I the atom has to enter the interval from the right, we obtain with

$$v \stackrel{(2.1)}{=} \frac{2m}{M+m} V' + \frac{M-m}{M+m} |V_1|$$

and $V' = -V_2 > 0$ the condition

$$\begin{aligned} \frac{2m}{M+m} V' + \frac{M-m}{M+m} |V_1| &< 0 \\ \Leftrightarrow |V_2| &< \frac{M-m}{M+m} |V_1|, \end{aligned}$$

such that $v < 0$. With $m < M \leq 2m$ we have that

$$\frac{M-m}{M+m} < \frac{3m-M}{M+m},$$

i.e. if we choose

$$|V_2| < \frac{M-m}{M+m} B,$$

we have to reduce τ in Scenario II, since (5.263) is not satisfied. As we outlined before, we have to restrict also the values for τ in Scenario I (cf. (5.256)). The restriction of τ in both scenarios leads to following arrival times τ_2 , which depend on V_1, τ_1 . In Scenario I we obtain that

$$\tau_1 + \frac{4L}{|V_1|} < \tau_2 < \tau_1 + \frac{4L}{|V_2|} \frac{M-m}{M+m}, \quad (5.275)$$

whereas in Scenario II we have that

$$\tau_1 + \frac{4L}{|V_2|} \frac{m}{M+m} < \tau_2 < \tau_1 + \frac{2L}{|V_1|} + \frac{2L}{|V_2|}. \quad (5.276)$$

To establish overlap, the r.h.s. of (5.275) has to be larger than the l.h.s. (5.276), i.e. for any τ_1, τ_1'

$$\tau_1 + \frac{4L}{|V_2|} \frac{m}{M+m} < \tau_1' + \frac{4L}{|V_2|} \frac{M-m}{M+m}. \quad (5.277)$$

Since $0 \leq \tau_1 \leq \frac{4L}{B}$, condition (5.277) is satisfied if

$$\begin{aligned} \frac{4L}{B} + \frac{4L}{|V_2|} \frac{m}{M+m} &< \frac{4L}{|V_2|} \frac{M-m}{M+m} \\ \Leftrightarrow \frac{4L}{B} &< \frac{4L}{|V_2|} \frac{M-2m}{M+m} \\ \Leftrightarrow |V_2| &< \frac{M-2m}{M+m} B. \end{aligned} \quad (5.278)$$

Since $m < M \leq 2m$, there are no values for V_2 such that (5.278) is satisfied, i.e. there is no overlap in respect to the arrival times τ_2 if we proceed as we just described.

We solve the difficulty of disjoint arrival times by redefining τ_2 as follows. Consider $Y(0) = y \in G_{B,C;0}$. If on $\mathcal{E}_{\tau_1(y)}$ (cf. (5.167)) $\sigma_1 = 1$, then denote by τ_2 the time the molecule is at L the second time after time $x = \frac{16L}{B} \frac{m}{M-m}$. If $\sigma_1 = -1$ τ_2 is the time the molecule is at L the second time after $t = 0$. By that, the values of τ_2 are shifted to the future if $\sigma_1 = 1$, such that similar arrival times as in Scenario II occur. Then, one can show that Lemma 5.7 holds for the redefined overlap set

$$O = \{\text{Molecule is alone at time } \tau_2, \quad (5.279)$$

$$V_2 \in \mathcal{V}_2 := \left(-\frac{B}{4} \frac{M-m}{M+m}, -\frac{B}{4} \frac{M-m}{M+m} \frac{M+7m}{2(M+3m)} \right), \quad (5.280)$$

$$\tau_2 \in \mathcal{T}_2 := \left[\frac{8L}{B} \frac{M+m}{M-m}, \frac{2L}{C} + \frac{8L}{B} \frac{M+m}{M-m} \right], \quad (5.281)$$

$$\sigma_2 = 1\}$$

with

$$\bar{\tau} = \frac{2L}{C} + \frac{8L}{B} \frac{M+m}{M-m} \quad (5.282)$$

and

$$g = \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\mathcal{K}m}{2} \left(\frac{M-m}{2m} C + \frac{M-m}{2m} \frac{B}{4} \right)^2} \left(\frac{M+m}{2m} \right)^2 \frac{B}{4} \frac{M-m}{M+m} \frac{M+7m}{2(M+3m)} e^{-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}}$$

(5.283)

with C given in (5.11).

The proof of Lemma 5.7 with the redefined sets O follow by similar arguments as Lemma 5.7 for $M > 3m$.

By the existence of an overlap set, which follows by (the redefined) Lemma 5.7, we can follow that transitions starting in $y_1, y_2 \in G_{B,C;0}$ are overlapping at time $\bar{\tau}$, which we show by the following lemma.

Lemma 5.8. Consider the Markov process \mathcal{M}_t (cf. (5.7)) with transition probability Π_y^t , $y \in \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$. Then, there exists a $\delta > 0$, which will be specified later, such that for $\bar{\tau}$ given in (5.242), (5.268), (5.273), (5.282) respectively,

$$\|\Pi_{y_1}^{\bar{\tau}} - \Pi_{y_2}^{\bar{\tau}}\| < 2(1 - \delta) \quad (5.284)$$

for any $y_1, y_2 \in G_{B,C;0}$ (cf. (5.12)).

Proof of Lemma 5.8. Note that the choice of $\bar{\tau}$ depends on $\frac{M}{m}$. Denote by

$$\mathcal{F}_{\bar{\tau}} := \sigma(Y(\bar{\tau}))$$

the σ -Algebra generated by $Y(\bar{\tau})$ and by $\mathbb{P}_y|_{\mathcal{F}_{\bar{\tau}}}$ the restriction of the path measure \mathbb{P}_y on $\mathcal{F}_{\bar{\tau}}$. Let $C \in \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$ be measurable, and denote by

$$A_{\bar{\tau},C} := \{Y(\omega) : Y(\omega, \bar{\tau}) \in C\}$$

the set of paths which are at time $\bar{\tau}$ in C . Then,

$$\mathbb{P}_y(A_{\bar{\tau},C}) = \Pi_y^{\bar{\tau}}(C) \quad (5.285)$$

and for the l.h.s. of (5.284) it follows that

$$\|\Pi_{y_1}^{\bar{\tau}} - \Pi_{y_2}^{\bar{\tau}}\| = 2 \sup_C |\Pi_{y_1}^{\bar{\tau}}(C) - \Pi_{y_2}^{\bar{\tau}}(C)| \quad (5.286)$$

$$\stackrel{(5.285)}{=} 2 \sup_C |\mathbb{P}_{y_1}(A_{\bar{\tau},C}) - \mathbb{P}_{y_2}(A_{\bar{\tau},C})|$$

$$= 2 \sup_{A \in \mathcal{F}_{\bar{\tau}}} |\mathbb{P}_{y_1}(A) - \mathbb{P}_{y_2}(A)|$$

$$= \|\mathbb{P}_{y_1}|_{\mathcal{F}_{\bar{\tau}}} - \mathbb{P}_{y_2}|_{\mathcal{F}_{\bar{\tau}}}\|. \quad (5.287)$$

To estimate (5.287) denote by

$$\bar{\mathbb{P}}_{y_1, y_2} |_{\mathcal{F}_{\bar{\tau}}} := \min\{\mathbb{P}_{y_1} |_{\mathcal{F}_{\bar{\tau}}}, \mathbb{P}_{y_2} |_{\mathcal{F}_{\bar{\tau}}}\} \quad (5.288)$$

the overlap measure of $\mathbb{P}_{y_1} |_{\mathcal{F}_{\bar{\tau}}}$ and $\mathbb{P}_{y_2} |_{\mathcal{F}_{\bar{\tau}}}$ with

$$\alpha_{y_1, y_2}^{\bar{\tau}} := \int \bar{\mathbb{P}}_{y_1, y_2} |_{\mathcal{F}_{\bar{\tau}}} (dY). \quad (5.289)$$

Then,

$$\underline{\mathbb{P}}_{y_1(y_2)} |_{\mathcal{F}_{\bar{\tau}}} := \mathbb{P}_{y_1} |_{\mathcal{F}_{\bar{\tau}}} - \bar{\mathbb{P}}_{y_1, y_2} |_{\mathcal{F}_{\bar{\tau}}} \quad (5.290)$$

and

$$\underline{\mathbb{P}}_{y_2(y_1)} |_{\mathcal{F}_{\bar{\tau}}} := \mathbb{P}_{y_2} |_{\mathcal{F}_{\bar{\tau}}} - \bar{\mathbb{P}}_{y_1, y_2} |_{\mathcal{F}_{\bar{\tau}}} \quad (5.291)$$

is the part of the measure $\mathbb{P}_{y_1} |_{\mathcal{F}_{\bar{\tau}}}$ resp. $\mathbb{P}_{y_2} |_{\mathcal{F}_{\bar{\tau}}}$ without overlap, i.e.

$$\int \underline{\mathbb{P}}_{y_1(y_2)} |_{\mathcal{F}_{\bar{\tau}}} (dY) = 1 - \alpha_{y_1, y_2}^{\bar{\tau}} = \int \underline{\mathbb{P}}_{y_2(y_1)} |_{\mathcal{F}_{\bar{\tau}}} (dY) \quad (5.292)$$

and $\underline{\mathbb{P}}_{y_1(y_2)} |_{\mathcal{F}_{\bar{\tau}}}, \underline{\mathbb{P}}_{y_2(y_1)} |_{\mathcal{F}_{\bar{\tau}}}$ are singular w.r.t. to each other. By that, (5.287) becomes

$$\|\mathbb{P}_{y_1} |_{\mathcal{F}_{\bar{\tau}}} - \mathbb{P}_{y_2} |_{\mathcal{F}_{\bar{\tau}}}\| = 2 \sup_{A \in \mathcal{F}_{\bar{\tau}}} |\mathbb{P}_{y_1}(A) - \mathbb{P}_{y_2}(A)| \quad (5.293)$$

$$\stackrel{(5.290), (5.291)}{=} 2 \sup_{A \in \mathcal{F}_{\bar{\tau}}} |\underline{\mathbb{P}}_{y_1}(A) - \underline{\mathbb{P}}_{y_2}(A)|$$

$$\stackrel{(5.292)}{=} 2(1 - \alpha_{y_1, y_2}^{\bar{\tau}}). \quad (5.294)$$

Since Lemma 5.8 requires a uniform upper bound, we now give a uniform lower bound for $\alpha_{y_1, y_2}^{\bar{\tau}}$ (cf. (5.289)), where we use (the redefined) Lemma 5.7. Note that τ_2 is a stopping time. Since the entrance of atoms into Λ may be described by a pure jump Markov process, which is a strong Markov process, \mathcal{M}_t has the strong Markov property, i.e. if τ_n is a stopping time, then

$$\mathbb{P}_y(dY(\cdot + \tau_n) | Y(t), t \leq \tau_n) = \mathbb{P}_{Y(\tau_n)}(dY).$$

Applying the strong Markov property to the stopping time τ_2 , we obtain for any $y \in G_{B, C; 0}$ that

$$\begin{aligned} \mathbb{P}_y |_{\mathcal{F}_{\bar{\tau}}}(dY) &= \mathbb{P}_y(dY(\bar{\tau})) \\ &= \int \mathbb{P}_y(d\tau_2, dY(\tau_2)) \mathbb{P}(dY(\bar{\tau}) | \tau_2, Y(\tau_2)) \\ &\geq \int_O \mathbb{P}_y(d\tau_2, dY(\tau_2)) \mathbb{P}(dY(\bar{\tau}) | \tau_2, Y(\tau_2)) \end{aligned} \quad (5.295)$$

with O given in (5.159), (5.265), (5.270), (5.279) respectively. Note that

$$\tau_2 < \bar{\tau}$$

on O since $\tau_2 \in \mathcal{T}_2$. By (the redefined) Lemma 5.7 we have that

$$(5.295) \stackrel{(5.163)}{\geq} g \cdot \int_{\mathcal{T}_2 \times \mathcal{V}_2} dV_2 d\tau_2 \mathbb{P}\left(dY(\bar{\tau})|_{\mathcal{T}_2}, Y(\tau_2) = (L, V_2, 1)\right), \quad (5.296)$$

with g given in (5.253), (5.269), (5.274), (5.283) respectively, \mathcal{V}_2 given in (5.160), (5.266), (5.271), (5.280) respectively, and \mathcal{T}_2 given in (5.161), (5.267), (5.272), (5.281) respectively. Since the r.h.s. of (5.296) is independent of y , we obtain for (5.289) by (5.295) and (5.296) that for any $y_1, y_2 \in G_{B,C;0}$

$$\alpha_{y_1, y_2}^{\bar{\tau}} \stackrel{(5.288)}{=} \int \min\{\mathbb{P}_{y_1}|_{\mathcal{F}_{\bar{\tau}}}, \mathbb{P}_{y_2}|_{\mathcal{F}_{\bar{\tau}}}\}(dY) \quad (5.297)$$

$$\geq \int g \cdot \int_{\mathcal{T}_2 \times \mathcal{V}_2} dV_2 d\tau_2 \mathbb{P}\left(dY(\bar{\tau})|_{\mathcal{T}_2}, Y(\tau_2) = (L, V_2, 1)\right). \quad (5.298)$$

To continue estimating, we define $\mathcal{E}_{\tau_2, \bar{\tau}} \subset \hat{\Omega}$ with

$$\mathcal{E}_{\tau_2, \bar{\tau}} := \{\text{No atom enters } \Lambda \text{ during } [\tau_2, \bar{\tau}]\},$$

and let $\mathcal{C}(\mathcal{E}_{\tau_2, \bar{\tau}})$ denote the corresponding set of paths, i.e. all paths for which $Y(\bar{\tau})$ is such as $\mathcal{E}_{\tau_2, \bar{\tau}}$ has happened. Then,

$$(5.298) \geq g \cdot \int_{\mathcal{T}_2 \times \mathcal{V}_2} dV_2 d\tau_2 \int_{\mathcal{C}(\mathcal{E}_{\tau_2, \bar{\tau}})} \mathbb{P}\left(dY(\bar{\tau})|_{\mathcal{T}_2}, Y(\tau_2) = (L, V_2, 1)\right) \\ \geq g \cdot \int_{\mathcal{T}_2 \times \mathcal{V}_2} dV_2 d\tau_2 \mu(\mathcal{E}_{\tau_2, \bar{\tau}}) \quad (5.299)$$

$$\stackrel{(5.22)}{=} g \cdot \int_{\mathcal{T}_2 \times \mathcal{V}_2} dV_2 d\tau_2 \exp\left(-\frac{2(\bar{\tau} - \tau_2)\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \\ > g \cdot \int_{\mathcal{T}_2 \times \mathcal{V}_2} dV_2 d\tau_2 \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right). \quad (5.300)$$

Note that (5.299) follows, since on $\mathcal{E}_{\tau_2, \bar{\tau}}$ the paths starting at τ_2 in $Y(\tau_2) = (L, V_2, 1)$ are in $\mathcal{C}(\mathcal{E}_{\tau_2, \bar{\tau}})$.

Since the set of \mathcal{V}_2 and \mathcal{T}_2 differ dependent on the mass of the molecule M , namely if $M > 3m$, $M = 3m$, $3m > M > 2m$ or $2m \geq M > m$, we continue estimating (5.300) depending on M .

If $M > 3m$, then \mathcal{V}_2 is given in (5.160) and \mathcal{T}_2 is given in (5.161). With that we obtain that

$$\int_{\mathcal{V}_2} dV_2 = \frac{M - 3m}{M + m} \frac{B}{5} - \frac{M - 3m}{M + 3m} \frac{B}{5}$$

$$= \frac{2m}{M+m} \frac{M-3m}{M+3m} \frac{B}{5} =: C_{V_2} \quad (5.301)$$

and

$$\int_{\mathcal{T}_2} d\tau_2 = \frac{10L}{B} \frac{M+m}{M-3m} - \frac{10L}{B} \frac{M}{M-3m} = \frac{10L}{B} \frac{m}{M-3m} =: C_{\tau_2}. \quad (5.302)$$

If $M = 3m$, \mathcal{V}_2 is given in (5.271) and \mathcal{T}_2 is given in (5.272), which gives

$$\int_{\mathcal{V}_2} dV_2 = \frac{B}{8} - \frac{B}{10} = \frac{B}{40} =: C_{V_2} \quad (5.303)$$

and

$$\int_{\mathcal{T}_2} d\tau_2 = \frac{16L}{B} - \frac{15L}{B} = \frac{L}{B} =: C_{\tau_2}. \quad (5.304)$$

If $3m > M > 2m$, then \mathcal{V}_2 is given in (5.266) and \mathcal{T}_2 is given in (5.267). With that it follows that

$$\begin{aligned} \int_{\mathcal{V}_2} dV_2 &= \frac{3m-M}{M+m} \frac{B}{2} - \frac{M}{2(M-m)} \frac{3m-M}{M+m} \frac{B}{2} \\ &= \frac{M-2m}{2(M-m)} \frac{3m-M}{M+m} \frac{B}{2} =: C_{V_2} \end{aligned} \quad (5.305)$$

and

$$\begin{aligned} \int_{\mathcal{T}_2} d\tau_2 &= \frac{4L}{B} + \frac{8L}{B} \frac{M-m}{3m-M} - \left(\frac{4L}{B} + \frac{8L}{B} \frac{2m}{M} \frac{M-m}{3m-M} \right) \\ &= \frac{8L}{B} \frac{M-m}{3m-M} \frac{M-2m}{M} =: C_{\tau_2}. \end{aligned} \quad (5.306)$$

If $2m \geq M > m$, then \mathcal{V}_2 is given in (5.280) and \mathcal{T}_2 is given in (5.281). This gives

$$\begin{aligned} \int_{\mathcal{V}_2} dV_2 &= \frac{M-m}{M+m} \frac{B}{4} - \frac{M+7m}{2(M+3m)} \frac{M-m}{M+m} \frac{B}{4} \\ &= \frac{M-m}{2(M+3m)} \frac{M-m}{M+m} \frac{B}{4} =: C_{V_2} \end{aligned} \quad (5.307)$$

and

$$\int_{\mathcal{T}_2} d\tau_2 = \frac{2L}{C} + \frac{8L}{B} \frac{M+m}{M-m} - \frac{8L}{B} \frac{M+m}{M-m} = \frac{2L}{C} =: C_{\tau_2}. \quad (5.308)$$

With these constants we have for (5.300) that

$$(5.300) = g \cdot \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \cdot C_{V_2} \cdot C_{\tau_2} \quad (5.309)$$

with the appropriate choice of g given in (5.253), (5.269), (5.274), (5.283) respectively, C_{V_2} given in (5.301), (5.303), (5.305), (5.307), respectively, and of C_{τ_2} given in (5.302), (5.304), (5.306), (5.308), respectively.

Altogether we have for (5.297) by (5.298), (5.300) and (5.309) that

$$\alpha_{y_1, y_2}^{\bar{\tau}} > g \cdot \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \cdot C_{V_2} \cdot C_{\tau_2}. \quad (5.310)$$

Finally, by (5.310) and (5.294) we obtain for (5.293) that

$$\|\mathbb{P}_{y_1}|_{\mathcal{F}_{\bar{\tau}}} - \mathbb{P}_{y_2}|_{\mathcal{F}_{\bar{\tau}}}\| < 2 \left(1 - g \cdot \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \cdot C_{V_2} \cdot C_{\tau_2}\right), \quad (5.311)$$

and by (5.311) and (5.287) for (5.286) that

$$\|\Pi_{y_1}^{\bar{\tau}} - \Pi_{y_2}^{\bar{\tau}}\| < 2 \left(1 - g \cdot \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \cdot C_{V_2} \cdot C_{\tau_2}\right).$$

Choosing

$$\delta = g \cdot \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \cdot C_{V_2} \cdot C_{\tau_2} \quad (5.312)$$

Lemma 5.8 follows. Note that $g > 0$ (cf. (5.253), (5.269), (5.274), (5.283) respectively), $C_{V_2} > 0$ (cf. (5.301), (5.303), (5.305), (5.307), respectively) and $C_{\tau_2} > 0$ (cf. (5.302), (5.304), (5.306), (5.308), respectively). \square

Finally, we prove the Overlap-Lemma 5.2 making use of Lemma 5.6 and Lemma 5.8.

Proof of Lemma 5.2. Let $y_1, y_2 \in G_{\bar{V}, \bar{N}}$ with $G_{\bar{V}, \bar{N}}$ given in (5.10). Since \mathcal{M}_t is a stationary Markov process, we have that

$$\|\Pi_{y_1}^{t(\bar{V}, \bar{N})+\bar{\tau}} - \Pi_{y_2}^{t(\bar{V}, \bar{N})+\bar{\tau}}\| = \left\| \int \Pi_{y_1}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) \Pi_y^{\bar{\tau}} - \int \Pi_{y_2}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) \Pi_y^{\bar{\tau}} \right\|, \quad (5.313)$$

with $t(\bar{V}, \bar{N})$ given in (5.129) and $\bar{\tau}$ in (5.242), (5.268), (5.273), (5.282) respectively. To make use of Lemma 5.8 it is useful to rename the integration variable y in (5.313) to y' in the subtrahend. With that and

$$\int \Pi_{\tilde{y}}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) = 1 \text{ for } \tilde{y} \in G_{\bar{V}, \bar{N}}, \quad (5.314)$$

it follows that

$$\begin{aligned}
(5.313) &= \left\| \int \Pi_{y_1}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) \Pi_y^{\bar{\tau}} - \int \Pi_{y_2}^{t(\bar{V}, \bar{N})}(\mathrm{d}y') \Pi_{y'}^{\bar{\tau}} \right\| \\
&\stackrel{(5.314)}{=} \left\| \int \Pi_{y_1}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) \int \Pi_{y_2}^{t(\bar{V}, \bar{N})}(\mathrm{d}y') (\Pi_y^{\bar{\tau}} - \Pi_{y'}^{\bar{\tau}}) \right\| \\
&\leq \int \Pi_{y_1}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) \int \Pi_{y_2}^{t(\bar{V}, \bar{N})}(\mathrm{d}y') \|\Pi_y^{\bar{\tau}} - \Pi_{y'}^{\bar{\tau}}\| \\
&= \int_{G_{B,C;0}} \Pi_{y_1}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) \int_{G_{B,C;0}} \Pi_{y_2}^{t(\bar{V}, \bar{N})}(\mathrm{d}y') \|\Pi_y^{\bar{\tau}} - \Pi_{y'}^{\bar{\tau}}\| + \\
&\quad + \int_{G_{B,C;0}} \Pi_{y_1}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) \int_{G_{B,C;0}^c} \Pi_{y_2}^{t(\bar{V}, \bar{N})}(\mathrm{d}y') \|\Pi_y^{\bar{\tau}} - \Pi_{y'}^{\bar{\tau}}\| + \\
&\quad + \int_{G_{B,C;0}^c} \Pi_{y_1}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) \int_{G_{B,C;0}} \Pi_{y_2}^{t(\bar{V}, \bar{N})}(\mathrm{d}y') \|\Pi_y^{\bar{\tau}} - \Pi_{y'}^{\bar{\tau}}\| + \\
&\quad + \int_{G_{B,C;0}^c} \Pi_{y_1}^{t(\bar{V}, \bar{N})}(\mathrm{d}y) \int_{G_{B,C;0}^c} \Pi_{y_2}^{t(\bar{V}, \bar{N})}(\mathrm{d}y') \|\Pi_y^{\bar{\tau}} - \Pi_{y'}^{\bar{\tau}}\|, \tag{5.315}
\end{aligned}$$

where $G_{B,C;0}^c$ is the complement of $G_{B,C;0}$. To continue estimating, we use Lemma 5.8, which gives in (5.315)

$$\|\Pi_y^{\bar{\tau}} - \Pi_{y'}^{\bar{\tau}}\| < 2(1 - \delta),$$

since $y, y' \in G_{B,C;0}$. Note that

$$\delta > 0.$$

To estimate $\|\Pi_y^{\bar{\tau}} - \Pi_{y'}^{\bar{\tau}}\|$ in the remaining summands we use the fact that the total variation distance of two probability measures is by definition bounded by 2 (cf. (5.2)). Altogether we obtain for (5.313) that

$$\begin{aligned}
\|\Pi_{y_1}^{t(\bar{V}, \bar{N})+\bar{\tau}} - \Pi_{y_2}^{t(\bar{V}, \bar{N})+\bar{\tau}}\| &< 2(1 - \delta) \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) + \\
&\quad + 2 \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0}^c) + \\
&\quad + 2 \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0}^c) \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) + \\
&\quad + 2 \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0}^c) \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0}^c) \\
&= 2(1 - \delta) \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) + \\
&\quad + 2 \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) (1 - \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0})) + \\
&\quad + 2(1 - \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0})) \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) + \\
&\quad + 2(1 - \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0})) (1 - \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0})) \\
&= \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) (2(1 - \delta) - 2) + 2 \\
&= 2 - 2 \Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) \Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B,C;0}) \delta. \tag{5.316}
\end{aligned}$$

Since by Lemma 5.6 for $y \in G_{\bar{V}, \bar{N}}$

$$\Pi_y^{t(\bar{V}, \bar{N})}(G_{B, C; 0}) \stackrel{(5.130)}{\geq} \varepsilon(\bar{V}, \bar{N}),$$

it follows that

$$\begin{aligned} (5.316) &= 2 - 2\Pi_{y_1}^{t(\bar{V}, \bar{N})}(G_{B, C; 0})\Pi_{y_2}^{t(\bar{V}, \bar{N})}(G_{B, C; 0})\delta \\ &\stackrel{(5.130)}{\leq} 2(1 - \varepsilon(\bar{V}, \bar{N})^2\delta) \\ &< 2. \end{aligned} \tag{5.317}$$

Note that (5.317) follows since $\varepsilon(\bar{V}, \bar{N}) > 0$ (cf. (5.131)) and $\delta > 0$ (cf. Lemma 5.8). The Overlap-Lemma 5.2 follows by choosing

$$\mathcal{G} = G_{\bar{V}, \bar{N}} \tag{5.318}$$

with $G_{\bar{V}, \bar{N}}$ given in (5.10),

$$t(\mathcal{G}) = t(\bar{V}, \bar{N}) + \bar{\tau}, \tag{5.319}$$

with $t(\bar{V}, \bar{N})$ given in (5.129) and $\bar{\tau}$ in (5.242), (5.268), (5.273) resp. (5.282) and

$$\gamma(\mathcal{G}) = 2(1 - \varepsilon(\bar{V}, \bar{N})^2\delta) \tag{5.320}$$

with $\varepsilon(\bar{V}, \bar{N}) > 0$ given in (5.131) and δ given in (5.312). \square

Using the overlap at time $t(\mathcal{G})$ of transitions starting in \mathcal{G} (cf. Overlap-Lemma 5.2), we get an estimate for the total variation distance for these transitions after multiples of $t(\mathcal{G})$. Since states of \mathcal{G} may leave this set, the distance will depend inter alia on the size of the complement of \mathcal{G} .

Corollary 5.1. Let \mathcal{G} , $t(\mathcal{G})$ and $\gamma(\mathcal{G})$ be from Overlap-Lemma 5.2. Then, for any $y_1, y_2 \in \mathcal{G}$ and $n \in \mathbb{N}_0$

$$\|\Pi_{y_1}^{(n+1)t(\mathcal{G})} - \Pi_{y_2}^{(n+1)t(\mathcal{G})}\| \leq \gamma_{n+1}(\mathcal{G}), \tag{5.321}$$

with

$$\gamma_{n+1}(\mathcal{G}) = 2 \left(\frac{\gamma(\mathcal{G})}{2} \right)^{n+1} + 4 \sum_{i=0}^{n-1} \left(\frac{\gamma(\mathcal{G})}{2} \right)^i \left(\Pi_{y_1}^{(n-i)t(\mathcal{G})}(\mathcal{G}^c) + \Pi_{y_2}^{(n-i)t(\mathcal{G})}(\mathcal{G}^c) \right), \tag{5.322}$$

where \mathcal{G}^c is the complement of \mathcal{G} . For $n = 0$ the sum taken over i in (5.322) is defined as zero.

Proof of Corollary 5.1. We prove Corollary 5.1 by induction. Let $\mathcal{G}, t(\mathcal{G})$ and $\gamma(\mathcal{G})$ be from Overlap-Lemma 5.2. Let $n = 0$, then (5.321) with (5.322) follows by the Overlap-Lemma 5.2.

In the induction step we show that for $y_1, y_2 \in \mathcal{G}$

$$\|\Pi_{y_1}^{nt(\mathcal{G})} - \Pi_{y_2}^{nt(\mathcal{G})}\| \leq \gamma_n(\mathcal{G}) \Rightarrow \|\Pi_{y_1}^{(n+1)t(\mathcal{G})} - \Pi_{y_2}^{(n+1)t(\mathcal{G})}\| \leq \gamma_{n+1}(\mathcal{G}) \quad (5.323)$$

with $\gamma_{n+1}(\mathcal{G})$ given in (5.322). We write in the following t for $t(\mathcal{G})$ and γ for $\gamma(\mathcal{G})$. To estimate

$$\|\Pi_{y_1}^{(n+1)t} - \Pi_{y_2}^{(n+1)t}\| = \left\| \int (\Pi_{y_1}^{nt} - \Pi_{y_2}^{nt})(dy) \Pi_y^t \right\|, \quad (5.324)$$

we make use of the overlap at time nt . Denote by α_{y_1, y_2}^{nt} with $0 \leq \alpha_{y_1, y_2}^{nt} \leq 1$ the overlap of $\Pi_{y_1}^{nt}, \Pi_{y_2}^{nt}$ and by

$$\bar{\Pi}_{y_1, y_2}^{nt} := \min\{\Pi_{y_1}^{nt}, \Pi_{y_2}^{nt}\}$$

the overlap measure of $\Pi_{y_1}^{nt}$ and $\Pi_{y_2}^{nt}$, i.e.

$$\alpha_{y_1, y_2}^{nt} := \int \bar{\Pi}_{y_1, y_2}^{nt}(dy).$$

Then,

$$\underline{\Pi}_{y_1(y_2)}^{nt} := \Pi_{y_1}^{nt} - \bar{\Pi}_{y_1, y_2}^{nt} \quad (5.325)$$

resp.

$$\underline{\Pi}_{y_2(y_1)}^{nt} := \Pi_{y_2}^{nt} - \bar{\Pi}_{y_1, y_2}^{nt} \quad (5.326)$$

is the part of the measure $\Pi_{y_1}^{nt}$ resp. $\Pi_{y_2}^{nt}$ without overlap, i.e.

$$\int \underline{\Pi}_{y_1(y_2)}^{nt}(dy) = 1 - \alpha_{y_1, y_2}^{nt} = \int \underline{\Pi}_{y_2(y_1)}^{nt}(dy) \quad (5.327)$$

and $\underline{\Pi}_{y_1(y_2)}^{nt}, \underline{\Pi}_{y_2(y_1)}^{nt}$ are singular w.r.t. to each other. By (5.325) and (5.326) we have that

$$\Pi_{y_1}^{nt} - \Pi_{y_2}^{nt} = \underline{\Pi}_{y_1(y_2)}^{nt} - \underline{\Pi}_{y_2(y_1)}^{nt}, \quad (5.328)$$

and using (5.328) and (5.327) it follows that

$$\begin{aligned} \|\Pi_{y_1}^{nt} - \Pi_{y_2}^{nt}\| &= \|\underline{\Pi}_{y_1(y_2)}^{nt} - \underline{\Pi}_{y_2(y_1)}^{nt}\| \\ &= 2 \sup_A \left| \int_A \underline{\Pi}_{y_1(y_2)}^{nt}(dy) - \int_A \underline{\Pi}_{y_2(y_1)}^{nt}(dy) \right| \end{aligned}$$

$$= 2(1 - \alpha_{y_1, y_2}^{nt}). \quad (5.329)$$

Note that by induction hypotheses for any $y_1, y_2 \in \mathcal{G}$

$$1 - \alpha_{y_1, y_2}^{nt} \leq \frac{\gamma_n}{2}. \quad (5.330)$$

For (5.324) and $y_1, y_2 \in \mathcal{G}$ we obtain by (5.328) that

$$\begin{aligned} \|\Pi_{y_1}^{(n+1)t} - \Pi_{y_2}^{(n+1)t}\| &= \left\| \int \left(\underline{\Pi}_{y_1(y_2)}^{nt} - \underline{\Pi}_{y_2(y_1)}^{nt} \right) (dy) \Pi_y^t \right\| \\ &= \left\| \int \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \Pi_y^t - \int \underline{\Pi}_{y_2(y_1)}^{nt} (dy) \Pi_y^t \right\|. \end{aligned} \quad (5.331)$$

To make use of (5.329) with (5.330) it is useful to rename the integration variable y in the subtrahend in (5.331) to y' . Now consider $\alpha_{y_1, y_2}^{nt} < 1$. With (5.327) it follows that

$$\int \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \Pi_y^t = \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int \underline{\Pi}_{y_2(y_1)}^{nt} (dy') \int \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \Pi_y^t \quad (5.332)$$

and similarly with interchanged y_1, y_2 . With that, (5.331) becomes

$$\begin{aligned} &\left\| \int \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \Pi_y^t - \int \underline{\Pi}_{y_2(y_1)}^{nt} (dy') \Pi_{y'}^t \right\| \\ &\stackrel{(5.332)}{=} \left\| \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int \underline{\Pi}_{y_2(y_1)}^{nt} (dy') \int \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \Pi_y^t - \right. \\ &\quad \left. - \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \int \underline{\Pi}_{y_2(y_1)}^{nt} (dy') \Pi_{y'}^t \right\| \\ &\leq \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \int \underline{\Pi}_{y_2(y_1)}^{nt} (dy') \|\Pi_y^t - \Pi_{y'}^t\|. \end{aligned} \quad (5.333)$$

Writing $\hat{\Omega}|_{\Lambda} \times \{-1, 1\} = \mathcal{G} \cup \mathcal{G}^c$ we obtain that

$$\begin{aligned} (5.333) &= \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int_{\mathcal{G}} \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \int_{\mathcal{G}} \underline{\Pi}_{y_2(y_1)}^{nt} (dy') \|\Pi_y^t - \Pi_{y'}^t\| + \\ &\quad + \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int_{\mathcal{G}^c} \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \int_{\mathcal{G}} \underline{\Pi}_{y_2(y_1)}^{nt} (dy') \|\Pi_y^t - \Pi_{y'}^t\| + \\ &\quad + \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int_{\mathcal{G}} \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \int_{\mathcal{G}^c} \underline{\Pi}_{y_2(y_1)}^{nt} (dy') \|\Pi_y^t - \Pi_{y'}^t\| + \\ &\quad + \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int_{\mathcal{G}^c} \underline{\Pi}_{y_1(y_2)}^{nt} (dy) \int_{\mathcal{G}^c} \underline{\Pi}_{y_2(y_1)}^{nt} (dy') \|\Pi_y^t - \Pi_{y'}^t\|. \end{aligned} \quad (5.334)$$

For the first summand in (5.334) we get by the Overlap-Lemma 5.2 and the monotonicity

of $\underline{\Pi}_y^{nt}$ that

$$\begin{aligned}
& \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int_{\mathcal{G}} \underline{\Pi}_{y_1(y_2)}^{nt}(dy) \int_{\mathcal{G}} \underline{\Pi}_{y_2(y_1)}^{nt}(dy') \|\Pi_y^t - \Pi_{y'}^t\| \\
& \stackrel{(5.9)}{\leq} \gamma \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \underline{\Pi}_{y_1(y_2)}^{nt}(\mathcal{G}) \underline{\Pi}_{y_2(y_1)}^{nt}(\mathcal{G}) \\
& \leq \gamma \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int \underline{\Pi}_{y_1(y_2)}^{nt}(dy) \int \underline{\Pi}_{y_2(y_1)}^{nt}(dy) \\
& \stackrel{(5.327)}{\leq} \gamma (1 - \alpha_{y_1, y_2}^{nt}) \\
& \stackrel{(5.330)}{\leq} \gamma \frac{\gamma_n}{2}. \tag{5.335}
\end{aligned}$$

Since the total variation distance is by definition bounded by 2 (cf. (5.2)), the second term in (5.334) is bounded by

$$\begin{aligned}
& \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int_{\mathcal{G}^c} \underline{\Pi}_{y_1(y_2)}^{nt}(dy) \int_{\mathcal{G}} \underline{\Pi}_{y_2(y_1)}^{nt}(dy') \|\Pi_y^t - \Pi_{y'}^t\| \\
& \leq 2 \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \underline{\Pi}_{y_1(y_2)}^{nt}(\mathcal{G}^c) \underline{\Pi}_{y_2(y_1)}^{nt}(\mathcal{G}) \\
& \leq 2 \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \underline{\Pi}_{y_1(y_2)}^{nt}(\mathcal{G}^c) \int \underline{\Pi}_{y_2(y_1)}^{nt}(dy) \\
& \stackrel{(5.327)}{\leq} 2 \underline{\Pi}_{y_1(y_2)}^{nt}(\mathcal{G}^c) \\
& \stackrel{(5.325)}{\leq} 2 \underline{\Pi}_{y_1}^{nt}(\mathcal{G}^c). \tag{5.336}
\end{aligned}$$

Similarly for the third term

$$\begin{aligned}
& \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int_{\mathcal{G}} \underline{\Pi}_{y_1(y_2)}^{nt}(dy) \int_{\mathcal{G}^c} \underline{\Pi}_{y_2(y_1)}^{nt}(dy') \|\Pi_y^t - \Pi_{y'}^t\| \\
& \leq 2 \underline{\Pi}_{y_2}^{nt}(\mathcal{G}^c), \tag{5.337}
\end{aligned}$$

while the fourth term can be estimated by

$$\begin{aligned}
& \frac{1}{1 - \alpha_{y_1, y_2}^{nt}} \int_{\mathcal{G}^c} \underline{\Pi}_{y_1(y_2)}^{nt}(dy) \int_{\mathcal{G}^c} \underline{\Pi}_{y_2(y_1)}^{nt}(dy') \|\Pi_y^t - \Pi_{y'}^t\| \\
& \leq \frac{2}{1 - \alpha_{y_1, y_2}^{nt}} \underline{\Pi}_{y_1(y_2)}^{nt}(\mathcal{G}^c) \underline{\Pi}_{y_2(y_1)}^{nt}(\mathcal{G}^c) \\
& \leq \frac{2}{1 - \alpha_{y_1, y_2}^{nt}} \int \underline{\Pi}_{y_1(y_2)}^{nt}(dy) \underline{\Pi}_{y_2(y_1)}^{nt}(\mathcal{G}^c) \\
& \stackrel{(5.327)}{\leq} 2 \underline{\Pi}_{y_2(y_1)}^{nt}(\mathcal{G}^c)
\end{aligned}$$

$$\stackrel{(5.326)}{\leq} 2\Pi_{y_2}^{nt}(\mathcal{G}^c). \quad (5.338)$$

Summing the upper bounds (5.335), (5.336), (5.337) and (5.338) of the summands in (5.334) it follows in total for (5.324) by (5.331), (5.333) and (5.334) that

$$\begin{aligned} \|\Pi_{y_1}^{(n+1)t} - \Pi_{y_2}^{(n+1)t}\| &\leq \gamma \frac{\gamma_n}{2} + 2\Pi_{y_1}^{nt}(\mathcal{G}^c) + 2\Pi_{y_2}^{nt}(\mathcal{G}^c) + 2\Pi_{y_2}^{nt}(\mathcal{G}^c) \\ &\leq \gamma \frac{\gamma_n}{2} + 4(\Pi_{y_1}^{nt}(\mathcal{G}^c) + \Pi_{y_2}^{nt}(\mathcal{G}^c)) \end{aligned} \quad (5.339)$$

with

$$\begin{aligned} &\frac{\gamma}{2}\gamma_n + 4(\Pi_{y_1}^{nt}(\mathcal{G}^c) + \Pi_{y_2}^{nt}(\mathcal{G}^c)) \\ &\stackrel{(5.322)}{=} \frac{\gamma}{2} \left(2 \left(\frac{\gamma}{2} \right)^n + 4 \sum_{i=0}^{n-2} \left(\frac{\gamma}{2} \right)^i \left(\Pi_{y_1}^{(n-i-1)t}(\mathcal{G}^c) + \Pi_{y_2}^{(n-i-1)t}(\mathcal{G}^c) \right) \right) + \\ &\quad + 4(\Pi_{y_1}^{nt}(\mathcal{G}^c) + \Pi_{y_2}^{nt}(\mathcal{G}^c)) \\ &= 2 \left(\frac{\gamma}{2} \right)^{n+1} + 4 \sum_{i=1}^{n-1} \left(\frac{\gamma}{2} \right)^i \left(\Pi_{y_1}^{(n-i)t}(\mathcal{G}^c) + \Pi_{y_2}^{(n-i)t}(\mathcal{G}^c) \right) + 4(\Pi_{y_1}^{nt}(\mathcal{G}^c) + \Pi_{y_2}^{nt}(\mathcal{G}^c)) \\ &\stackrel{(5.322)}{=} \gamma_{n+1}. \end{aligned} \quad (5.340)$$

Note that we considered underneath (5.331) that $\alpha_{y_1, y_2}^{nt} < 1$. Let now $\alpha_{y_1, y_2}^{nt} = 1$. This yields in (5.331) that

$$\|\Pi_{y_1}^{(n+1)t} - \Pi_{y_2}^{(n+1)t}\| = \left\| \int \underline{\Pi}_{y_1(y_2)}^{nt}(\mathrm{d}y) \Pi_y^t - \int \underline{\Pi}_{y_2(y_1)}^{nt}(\mathrm{d}y) \Pi_y^t \right\| \stackrel{(5.327)}{=} 0. \quad (5.341)$$

By (5.339), (5.340) and (5.341) we obtain (5.323) which ends the proof of Corollary 5.1. \square

By the Overlap-Lemma 5.2 and Corollary 5.1 we obtain an estimate for $\beta(t)$ (cf. (5.4)).

Corollary 5.2. Let $\mathcal{G}, t(\mathcal{G})$ and $\gamma(\mathcal{G})$ be from Overlap-Lemma 5.2 and $\beta(t)$ as given in (5.4). Then,

$$\beta((n+1)t(\mathcal{G})) \leq 2 \left(\frac{\gamma(\mathcal{G})}{2} \right)^{n+1} + 8(n+1)\Pi(\mathcal{G}^c). \quad (5.342)$$

Proof of Corollary 5.2. By Corollary 5.1 and using that for the stationary distribution

$$\Pi = \int \Pi(\mathrm{d}y) \Pi_y^t, \text{ for any } t, \quad (5.343)$$

we estimate the l.h.s. of (5.342).

$$\beta((n+1)t(\mathcal{G})) \stackrel{(5.4)}{=} \int \Pi(dy) \|\Pi_y^{(n+1)t(\mathcal{G})} - \Pi\| \quad (5.344)$$

$$\begin{aligned} & \stackrel{(5.343)}{=} \int \Pi(dy) \left\| \Pi_y^{(n+1)t(\mathcal{G})} - \int \Pi(dy') \Pi_{y'}^{(n+1)t(\mathcal{G})} \right\| \\ & = \int \Pi(dy) \left\| \int \Pi(dy') \left(\Pi_y^{(n+1)t(\mathcal{G})} - \Pi_{y'}^{(n+1)t(\mathcal{G})} \right) \right\| \\ & \leq \int \Pi(dy) \int \Pi(dy') \|\Pi_y^{(n+1)t(\mathcal{G})} - \Pi_{y'}^{(n+1)t(\mathcal{G})}\|. \end{aligned} \quad (5.345)$$

Since Corollary 5.1 applies to transitions starting in \mathcal{G} , we again write $\hat{\Omega}|_{\Lambda} \times \{-1, 1\} = \mathcal{G} \cup \mathcal{G}^c$ and split the integrals. Hence,

$$\begin{aligned} (5.345) & \leq \int_{\mathcal{G}} \Pi(dy) \int_{\mathcal{G}} \Pi(dy') \|\Pi_y^{(n+1)t(\mathcal{G})} - \Pi_{y'}^{(n+1)t(\mathcal{G})}\| + \\ & \quad + \int_{\mathcal{G}} \Pi(dy) \int_{\mathcal{G}^c} \Pi(dy') \|\Pi_y^{(n+1)t(\mathcal{G})} - \Pi_{y'}^{(n+1)t(\mathcal{G})}\| + \\ & \quad + \int_{\mathcal{G}^c} \Pi(dy) \int_{\mathcal{G}} \Pi(dy') \|\Pi_y^{(n+1)t(\mathcal{G})} - \Pi_{y'}^{(n+1)t(\mathcal{G})}\| + \\ & \quad + \int_{\mathcal{G}^c} \Pi(dy) \int_{\mathcal{G}^c} \Pi(dy') \|\Pi_y^{(n+1)t(\mathcal{G})} - \Pi_{y'}^{(n+1)t(\mathcal{G})}\|. \end{aligned} \quad (5.346)$$

To continue estimating we use

$$\int_{\mathcal{G}} \Pi(dy) \leq 1$$

and for the first term in (5.346) we use Corollary 5.1, while for the second, third and fourth term we use that the total variation distance is bounded by 2 (cf. (5.2)). This yields

$$\begin{aligned} (5.346) & \stackrel{(5.321)}{\leq} 2 \left(\frac{\gamma(\mathcal{G})}{2} \right)^{n+1} + \\ & \quad + 4 \sum_{i=0}^{n-1} \left(\frac{\gamma(\mathcal{G})}{2} \right)^i \int \Pi(dy) \int \Pi(dy') \left(\Pi_y^{(n-i)t(\mathcal{G})}(\mathcal{G}^c) + \Pi_{y'}^{(n-i)t(\mathcal{G})}(\mathcal{G}^c) \right) + \\ & \quad + 2\Pi(\mathcal{G})\Pi(\mathcal{G}^c) + 2\Pi(\mathcal{G}^c)\Pi(\mathcal{G}) + 2\Pi(\mathcal{G}^c)\Pi(\mathcal{G}^c) \\ & \leq 2 \left(\frac{\gamma(\mathcal{G})}{2} \right)^{n+1} + 4 \sum_{i=0}^{n-1} \left(\frac{\gamma(\mathcal{G})}{2} \right)^i \left(\int \Pi(dy') \int \Pi(dy) \Pi_y^{(n-i)t(\mathcal{G})}(\mathcal{G}^c) + \right. \\ & \quad \left. + \int \Pi(dy) \int \Pi(dy') \Pi_{y'}^{(n-i)t(\mathcal{G})}(\mathcal{G}^c) \right) + 6\Pi(\mathcal{G}^c) \\ & \stackrel{(5.343)}{=} 2 \left(\frac{\gamma(\mathcal{G})}{2} \right)^{n+1} + 8\Pi(\mathcal{G}^c) \sum_{i=0}^{n-1} \left(\frac{\gamma(\mathcal{G})}{2} \right)^i + 6\Pi(\mathcal{G}^c). \end{aligned} \quad (5.347)$$

Since $\frac{\gamma(\mathcal{G})}{2} < 1$, it follows that

$$\sum_{i=0}^{n-1} \left(\frac{\gamma(\mathcal{G})}{2} \right)^i < \sum_{i=0}^{n-1} 1 = n. \quad (5.348)$$

We finally have for (5.344) by (5.345), (5.346), (5.347) and (5.348) that

$$\beta((n+1)t(\mathcal{G})) \leq 2 \left(\frac{\gamma(\mathcal{G})}{2} \right)^{n+1} + 8(n+1)\Pi(\mathcal{G}^c).$$

□

Since in the proof of Overlap-Lemma 5.2 we showed that the set $G_{\bar{V}, \bar{N}}$ (cf. (5.10)) with $t(G_{\bar{V}, \bar{N}})$ (cf. (5.319)) and $\gamma(G_{\bar{V}, \bar{N}})$ (cf. (5.320)) fulfills the condition of the Overlap-Lemma 5.2, we obtain by Corollary 5.2 the estimate (5.342) for $\beta((n+1)t(G_{\bar{V}, \bar{N}}))$. To prove Proposition 5.1, we have to set $G_{\bar{V}, \bar{N}}$, i.e. \bar{V}, \bar{N} , in dependence of n , and show that there is a choice of $\bar{V}(n)$ and $\bar{N}(n)$, such that for $n \rightarrow \infty$ $\Pi(G_{\bar{V}(n), \bar{N}(n)}^c)$ approaches zero fast enough and $\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)})}{2}$ approaches one slow enough. If there is such a choice, we obtain at the end a good estimate for $\beta(t)$, which means that by the estimate we can show that $\beta(t) \rightarrow 0$ fast enough with $t \rightarrow \infty$ such that Proposition 5.1 can be proven. The following lemma is about a “good choice” of $\bar{V}(n)$ and $\bar{N}(n)$.

Lemma 5.9. Let $n \in \mathbb{N}$. Consider the set $G_{\bar{V}(n), \bar{N}(n)} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$, which is $G_{\bar{V}, \bar{N}}$ as defined in (5.10), but where \bar{V}, \bar{N} are functions of n . Let $t(G_{\bar{V}(n), \bar{N}(n)})$, $\gamma(G_{\bar{V}(n), \bar{N}(n)})$ as given in (5.319) resp. (5.320), but with $\bar{V}(n), \bar{N}(n)$ instead of \bar{V}, \bar{N} . Then, there exist $N \in \mathbb{N}$, and increasing unbounded functions $\bar{N}(n), \bar{V}(n), i(n)$, which will be specified later, and constants A_1, A_2 such that for all $n > N$

$$\beta(i(n)) < \beta((n+1)t(G_{\bar{V}(n), \bar{N}(n)})) \quad (5.349)$$

and

$$2 \left(\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)})}{2} \right)^{n+1} + 8(n+1)\Pi(G_{\bar{V}(n), \bar{N}(n)}^c) < 2 \exp(-A_1 i(n)^{\frac{2}{5}}) + A_2 i(n)^{-4}. \quad (5.350)$$

Note since $G_{\bar{V}(n), \bar{N}(n)}$ satisfies the conditions of the Overlap-Lemma 5.2 (see (5.318)), by Corollary 5.2 inequality (5.342) holds for $\mathcal{G} = G_{\bar{V}(n), \bar{N}(n)}$, so that the r.h.s. of (5.349) is smaller than the l.h.s. of (5.350).

Proof of Lemma 5.9. We first show that there exist $\tilde{N} \in \mathbb{N}$, increasing unbounded func-

tions $\bar{V}(n)$ and $\bar{N}(n)$ and a constant C_{14} such that for all $n > \tilde{N}$

$$\Pi\left(G_{\bar{V}(n), \bar{N}(n)}^c\right) \leq \frac{C_{14}}{8}(n+1)^{-6}, \quad (5.351)$$

where $G_{\bar{V}(n), \bar{N}(n)}^c$ is the complement of $G_{\bar{V}(n), \bar{N}(n)}$.
Since

$$\begin{aligned} G_{\bar{V}(n), \bar{N}(n)}^c = & \{|V| > \bar{V}(n)\} \cup \{N > \bar{N}(n)\} \cup \\ & \cup \{1 \leq N \leq \bar{N}(n), \exists j \in \{1, \dots, N\} : |v_j| \geq \bar{V}(n)\}, \end{aligned}$$

we can estimate the l.h.s. of (5.351) by

$$\begin{aligned} \Pi\left(G_{\bar{V}(n), \bar{N}(n)}^c\right) \leq & \Pi(\{N > \bar{N}(n)\}) + \Pi(\{|V| > \bar{V}(n)\}) + \\ & + \Pi(\{1 \leq N \leq \bar{N}(n), \exists j \in \{1, \dots, N\} : |v_j| \geq \bar{V}(n)\}). \end{aligned}$$

Inequality (5.351) follows as soon as we can find \tilde{N} , $\bar{V}(n)$, $\bar{N}(n)$, C_{14} such that for all $n > \tilde{N}$

$$\Pi(\{N > \bar{N}(n)\}) \leq \frac{1}{2} \frac{C_{14}}{8}(n+1)^{-6} \quad (5.352)$$

and

$$\Pi(\{|V| > \bar{V}(n)\}) + \Pi(\{1 \leq N \leq \bar{N}(n), \exists j \in \{1, \dots, N\} : |v_j| \geq \bar{V}(n)\}) \leq \quad (5.353)$$

$$\leq \frac{1}{2} \frac{C_{14}}{8}(n+1)^{-6}. \quad (5.354)$$

First, we determine $\bar{N}(n)$ and make demands on C_{14} and \tilde{N} such that (5.352) is satisfied for all $n > \tilde{N}$. The equilibrium distribution for the atoms in Λ is Poisson with parameter ρ (cf. (2.6)), hence, by Stirling's formular ($N! > \sqrt{2\pi}e^{-N+N \ln N}$)

$$\Pi(\{N > \bar{N}(n)\}) = \sum_{N=\bar{N}(n)+1}^{\infty} e^{-2L\rho} \frac{(2L\rho)^N}{N!} \quad (5.355)$$

$$\begin{aligned} & \leq \sum_{N=\bar{N}(n)}^{\infty} \frac{e^{-2L\rho}}{\sqrt{2\pi}} e^{N-N \ln(N)+N \ln(2L\rho)} \\ & = \frac{e^{-2L\rho}}{\sqrt{2\pi}} \sum_{N=\bar{N}(n)}^{\infty} \left(e^{1-\ln(N)+\ln(2L\rho)}\right)^N \\ & < \frac{e^{-2L\rho}}{\sqrt{2\pi}} \sum_{N=\bar{N}(n)}^{\infty} \left(e^{1-\ln(\bar{N}(n))+\ln(2L\rho)}\right)^N. \end{aligned} \quad (5.356)$$

There exists $N_1 \in \mathbb{N}$ such that for all $n > N_1$ $\bar{N}(n)$ (which is by definition an increasing

unbounded function) is large enough, such that

$$1 - \ln(\bar{N}(n)) + \ln(2L\rho) < -1,$$

i.e.

$$e^{1 - \ln(\bar{N}(n)) + \ln(2L\rho)} < \frac{1}{2}. \quad (5.357)$$

Hence, for $n > N_1$ (5.356) is a geometric series and

$$\begin{aligned} \sum_{N=\bar{N}(n)} \left(e^{1 - \ln(\bar{N}(n)) + \ln(2L\rho)} \right)^N &= \\ &= \sum_{N=0} \left(e^{1 - \ln(\bar{N}(n)) + \ln(2L\rho)} \right)^N - \sum_{N=0}^{\bar{N}(n)-1} \left(e^{1 - \ln(\bar{N}(n)) + \ln(2L\rho)} \right)^N \\ (5.357) \quad &= \frac{1}{1 - e^{1 - \ln(\bar{N}(n)) + \ln(2L\rho)}} - \frac{1 - \left(e^{1 - \ln(\bar{N}(n)) + \ln(2L\rho)} \right)^{\bar{N}(n)}}{1 - e^{1 - \ln(\bar{N}(n)) + \ln(2L\rho)}} \\ &= \frac{e^{\bar{N}(n) - \bar{N}(n) \ln(\bar{N}(n)) + \bar{N}(n) \ln(2L\rho)}}{1 - e^{1 - \ln(\bar{N}(n)) + \ln(2L\rho)}} \\ (5.357) \quad &\leq \frac{e^{\bar{N}(n) - \bar{N}(n) \ln(\bar{N}(n)) + \bar{N}(n) \ln(2L\rho)}}{1 - \frac{1}{2}} \\ &= 2e^{\bar{N}(n) - \bar{N}(n) \ln(\bar{N}(n)) + \bar{N}(n) \ln(2L\rho)} \\ &= 2e^{-\bar{N}(n) (\ln(\bar{N}(n)) - 1 - \ln(2L\rho))}, \end{aligned} \quad (5.358)$$

and for (5.355) it follows by (5.356) and (5.358) that

$$\Pi(\{N > \bar{N}(n)\}) \leq 2 \frac{e^{-2L\rho}}{\sqrt{2\pi}} e^{-\bar{N}(n) (\ln(\bar{N}(n)) - 1 - \ln(2L\rho))}. \quad (5.359)$$

Choose now

$$\bar{N}(n) = \frac{\ln(n+1)}{4(C_3 + C_{13})} \quad (5.360)$$

with C_3, C_{13} given in (5.44) resp. (5.135). Note that $C_3 + C_{13}$ will occur in (5.377). Plugging (5.360) into the exponent in (5.359) gives for the exponent that

$$\begin{aligned} -\bar{N}(n) (\ln(\bar{N}(n)) - 1 - \ln(2L\rho)) &= \\ (5.360) \quad &= -\frac{\ln(n+1)}{4(C_3 + C_{13})} \left(\ln \left(\frac{\ln(n+1)}{4(C_3 + C_{13})} \right) - 1 - \ln(2L\rho) \right). \end{aligned} \quad (5.361)$$

Since there exists $N_2 \in \mathbb{N}$ such that for all $n > N_2$

$$(5.361) < -6 \ln(n+1) ,$$

we obtain for (5.359) by the choice (5.360) and $n > N_2$ that

$$\begin{aligned} \Pi(\{N > \bar{N}(n)\}) &\leq 2 \frac{e^{-2L\rho}}{\sqrt{2\pi}} e^{-\bar{N}(n)(\ln(\bar{N}(n))-1-\ln(2L\rho))} \\ &< 2 \frac{e^{-2L\rho}}{\sqrt{2\pi}} e^{-6 \ln(n+1)} \\ &= 2 \frac{e^{-2L\rho}}{\sqrt{2\pi}} (n+1)^{-6} . \end{aligned}$$

(5.352) follows for any $C_{14} > 32 \frac{e^{-2L\rho}}{\sqrt{2\pi}}$ and any $\tilde{N} > \max\{N_1, N_2\}$.

Second, we determine the function $\bar{V}(n)$ and make demands on C_{14} and \tilde{N} such that with the choice (5.360) inequality (5.354) is satisfied for all $n > \tilde{N}$. The equilibrium distribution for the velocity of the atoms and the molecule is the Maxwellian given in (2.5) resp. (2.8). Since $\bar{V}(n)$ is by definition an increasing unbounded function, there exists $N_3 \in \mathbb{N}$ such that for all $n > N_3$ $\bar{V}(n)$ is large enough such that

$$\left(\frac{\mathcal{K}M}{2\pi}\right)^{\frac{1}{2}} \int_{\bar{V}(n)}^{\infty} e^{-\frac{\mathcal{K}M}{2}V^2} dV \leq \left(\frac{\mathcal{K}M}{2\pi}\right)^{\frac{1}{2}} \int_{\bar{V}(n)}^{\infty} V e^{-\frac{\mathcal{K}M}{2}V^2} dV = \frac{e^{-\frac{\mathcal{K}M}{2}\bar{V}(n)^2}}{\sqrt{2\pi\mathcal{K}M}} , \quad (5.362)$$

and similar for m instead of M . Then, for first summand in (5.353) we get for $n > N_3$ that

$$\Pi(\{|V| > \bar{V}(n)\}) = 2 \left(\frac{\mathcal{K}M}{2\pi}\right)^{\frac{1}{2}} \int_{\bar{V}(n)}^{\infty} e^{-\frac{\mathcal{K}M}{2}V^2} dV \stackrel{(5.362)}{\leq} 2 \frac{e^{-\frac{\mathcal{K}M}{2}\bar{V}(n)^2}}{\sqrt{2\pi\mathcal{K}M}} . \quad (5.363)$$

The second summand in (5.353) we estimate as follows.

$$\Pi(\{1 \leq N \leq \bar{N}(n), \exists j \in \{1, \dots, N\} : |v_j| \geq \bar{V}(n)\}) \quad (5.364)$$

$$\begin{aligned} &= \sum_{l=1}^{\bar{N}(n)} \Pi(\{\exists j \in \{1, \dots, N\} : |v_j| \geq \bar{V}(n)\} \{N = l\}) \Pi(\{N = l\}) \\ &\leq \sum_{l=1}^{\bar{N}(n)} \sum_{k=1}^l \Pi(\{|v_{n_1}| \geq \bar{V}(n), \dots, |v_{n_k}| \geq \bar{V}(n), n_i \in \{1, \dots, l\}\}) . \end{aligned} \quad (5.365)$$

Since each atom is given initially a random velocity according to the Maxwell distribution independently of its position and the other atoms, it follows that

$$(5.365) = \sum_{l=1}^{\bar{N}(n)} \sum_{k=1}^l \binom{l}{k} \Pi(\{|v_1| \geq \bar{V}(n), \dots, |v_k| \geq \bar{V}(n)\})$$

$$\begin{aligned}
&= \sum_{l=1}^{\bar{N}(n)} \sum_{k=1}^l \binom{l}{k} \Pi(\{|v_1| > \bar{V}(n)\})^k \\
&\leq \sum_{l=1}^{\bar{N}(n)} \sum_{k=1}^l \binom{l}{k} \Pi(\{|v_1| > \bar{V}(n)\}) \\
&= \sum_{l=1}^{\bar{N}(n)} (2^l - 1) \Pi(\{|v_1| > \bar{V}(n)\}) \\
&< \sum_{l=1}^{\bar{N}(n)} (2^{\bar{N}(n)} - 1) \Pi(\{|v_1| > \bar{V}(n)\}) \\
&\stackrel{(5.362)}{\leq} \bar{N}(n)(2^{\bar{N}(n)} - 1)2(2\pi\mathcal{K}m)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}m}{2}\bar{V}(n)^2}. \tag{5.366}
\end{aligned}$$

By (5.363) and (5.366), which is the estimate for (5.364), we obtain for (5.353) that

$$\Pi(\{|V| > \bar{V}(n)\}) + \Pi(\{1 \leq N \leq \bar{N}(n), \exists j \in \{1, \dots, N\} : |v_j| \geq \bar{V}(n)\}) < \tag{5.367}$$

$$\begin{aligned}
&< 2(2\pi\mathcal{K}M)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}M}{2}\bar{V}(n)^2} + \bar{N}(n)2(2^{\bar{N}(n)} - 1)(2\pi\mathcal{K}m)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}m}{2}\bar{V}(n)^2} \\
&\stackrel{M > m}{\leq} (1 + \bar{N}(n)(2^{\bar{N}(n)} - 1))2(2\pi\mathcal{K}m)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}m}{2}\bar{V}(n)^2} \\
&\leq 2\bar{N}(n)(2^{\bar{N}(n)} - 1)2(2\pi\mathcal{K}m)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}m}{2}\bar{V}(n)^2} \\
&\leq 2\bar{N}(n)2^{\bar{N}(n)}2(2\pi\mathcal{K}m)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}m}{2}\bar{V}(n)^2} \tag{5.368}
\end{aligned}$$

$$\begin{aligned}
&\stackrel{(5.360)}{=} \frac{\ln(n+1)}{4(C_3 + C_{13})} 2^{\frac{\ln(n+1)}{4(C_3 + C_{13})}} 4(2\pi\mathcal{K}m)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}m}{2}\bar{V}(n)^2} \\
&\leq \frac{\ln(n+1)}{(C_3 + C_{13})} (n+1)^{\frac{1}{4(C_3 + C_{13})}} (2\pi\mathcal{K}m)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}m}{2}\bar{V}(n)^2}. \tag{5.369}
\end{aligned}$$

Since there exists $N_4 \in \mathbb{N}$ such that for all $n > N_4$

$$\frac{\ln(n+1)}{(C_3 + C_{13})} < (n+1)^{\frac{1}{4(C_3 + C_{13})}},$$

(5.369) can be estimated by

$$(5.369) \leq (n+1)^{\frac{2}{4(C_3 + C_{13})}} (2\pi\mathcal{K}m)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}m}{2}\bar{V}(n)^2}. \tag{5.370}$$

Choosing

$$\bar{V}(n) = \left(\frac{4 \left(12 + \frac{1}{C_3 + C_{13}} \right) \ln(n+1)}{\mathcal{K}m} \right)^{\frac{1}{2}} \tag{5.371}$$

we have that

$$\begin{aligned} -\frac{\mathcal{K}m}{2}\bar{V}(n)^2 &\stackrel{(5.371)}{=} -2\left(12 + \frac{1}{C_3 + C_{13}}\right)\ln(n+1) \\ &< -\left(6 + \frac{1}{2(C_3 + C_{13})}\right)\ln(n+1). \end{aligned} \quad (5.372)$$

This gives for (5.370) that

$$\begin{aligned} (5.370) &= (n+1)^{\frac{2}{4(C_3+C_{13})}}(2\pi\mathcal{K}m)^{-\frac{1}{2}}e^{-\frac{\mathcal{K}m}{2}\bar{V}(n)^2} \\ &\stackrel{(5.372)}{\leq} (n+1)^{\frac{2}{4(C_3+C_{13})}}(2\pi\mathcal{K}m)^{-\frac{1}{2}}(n+1)^{-\left(6+\frac{1}{2(C_3+C_{13})}\right)} \\ &= (2\pi\mathcal{K}m)^{-\frac{1}{2}}(n+1)^{-6}. \end{aligned} \quad (5.373)$$

Altogether we have for (5.367) with (5.371) by (5.369), (5.370), (5.372) and (5.373) for all $n > \max\{N_3, N_4\}$ that

$$\begin{aligned} \Pi(\{|V| > \bar{V}(n)\}) + \Pi(\{1 \leq N \leq \bar{N}(n), \exists j \in \{1, \dots, N\} : |v_j| \geq \bar{V}(n)\}) &< \\ &< (2\pi\mathcal{K}m)^{-\frac{1}{2}}(n+1)^{-6}. \end{aligned}$$

Hence, choosing (5.371), inequality (5.354) is satisfied if $C_{14} > 16(2\pi\mathcal{K}m)^{-\frac{1}{2}}$ and $\tilde{N} > \max\{N_3, N_4\}$.

All in all (5.351) follows by choosing $\bar{N}(n)$ as given in (5.360), $\bar{V}(n)$ as given in (5.371), for all $n > \tilde{N}$ with

$$\tilde{N} = \max\{N_1, N_2, N_3, N_4\} \quad (5.374)$$

and

$$C_{14} = 32 \left(\frac{e^{-2L\rho}}{\sqrt{2\pi}} + (\sqrt{2\pi\mathcal{K}m})^{-1} \right). \quad (5.375)$$

To obtain Lemma 5.9 we now show, using (5.351), that the choice we made for $\bar{N}(n)$ and $\bar{V}(n)$, namely (5.360) resp. (5.371), gives $\gamma(G_{\bar{V}(n), \bar{N}(n)})$ and $t(G_{\bar{V}(n), \bar{N}(n)})$ such that there is a $i(n)$ for which the inequalities in Lemma 5.9 holds for n large enough.

First, we determine $\gamma(G_{\bar{V}(n), \bar{N}(n)})$ and $t(G_{\bar{V}(n), \bar{N}(n)})$. By the definition of $\gamma(G_{\bar{V}(n), \bar{N}(n)})$ (cf. (5.320)) we have that

$$\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)})}{2} = 1 - \varepsilon(\bar{V}(n), \bar{N}(n))^2 \delta. \quad (5.376)$$

Recall that

$$\begin{aligned} \varepsilon(\bar{V}(n), \bar{N}(n)) &\stackrel{(5.131)}{=} \\ &= \min\{C_{10}e^{-C_{11}\bar{V}(n)}, C_{12}e^{-C_{13}\bar{N}(n)}\} \cdot \min\{C_1C_4e^{-C_5\bar{V}(n)}, C_1C_2e^{-C_3\bar{N}(n)}\}. \end{aligned}$$

With the choices (5.360) and (5.371) there exists $N_5 \in \mathbb{N}$ such that for any $n > N_5$

$$\min\{C_{10}e^{-C_{11}\bar{V}(n)}, C_{12}e^{-C_{13}\bar{N}(n)}\} = C_{12}e^{-C_{13}\bar{N}(n)}$$

and

$$\min\{C_1C_4e^{-C_5\bar{V}(n)}, C_1C_2e^{-C_3\bar{N}(n)}\} = C_1C_2e^{-C_3\bar{N}(n)},$$

and we obtain that for $n > N_5$

$$\varepsilon(\bar{V}(n), \bar{N}(n)) = C_1C_2C_{12}e^{-(C_3+C_{13})\bar{N}(n)}.$$

Plugging that into (5.376) gives for $n > N_5$

$$\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)})}{2} = 1 - (C_1C_2C_{12})^2 e^{-2(C_3+C_{13})\bar{N}(n)} \delta \quad (5.377)$$

$$\begin{aligned} &\stackrel{(5.360)}{=} 1 - \delta(C_1C_2C_{12})^2 (n+1)^{-\frac{1}{2}} \\ &= 1 - C_{15}(n+1)^{-\frac{1}{2}} \end{aligned} \quad (5.378)$$

with

$$\begin{aligned} C_{15} &:= \delta(C_1C_2C_{12})^2 \\ &\stackrel{(5.18), (5.43), (5.134)}{=} \frac{\delta}{4} \exp\left(-\frac{4\rho\left(\frac{24L}{B} + 3\left(\rho \int_{D_b}^{D_c} v f(v) dv\right)^{-1}\right)}{\sqrt{2\pi\mathcal{K}m}}\right), \end{aligned} \quad (5.379)$$

and D_b, D_c given in (5.25), $\delta > 0$ (cf. Lemma 5.8).

Now we determine $t(G_{\bar{V}(n), \bar{N}(n)})$ (cf. (5.319)) for the choices (5.360) and (5.371) and give an estimate. Recall that

$$t(G_{\bar{V}(n), \bar{N}(n)}) \stackrel{(5.319)}{=} t(\bar{V}(n), \bar{N}(n)) + \bar{\tau} \quad (5.380)$$

and that

$$\begin{aligned} t(\bar{V}(n), \bar{N}(n)) &\stackrel{(5.129)}{=} \max\{4t_B + t(\bar{V}), 4t_B + t(\bar{N})\} \\ &\stackrel{(5.139), (5.143)}{=} \max\{C_6 + C_7\bar{V}(n), C_8 + C_9\bar{N}(n)\}. \end{aligned} \quad (5.381)$$

Since (5.360) and (5.371), there exists $N_6 \in \mathbb{N}$ such that for any $n > N_6$

$$(5.381) = C_8 + C_9 \bar{N}(n) \stackrel{(5.360)}{=} C_8 + \frac{C_9}{4(C_3 + C_{13})} \ln(n+1),$$

so that we obtain for (5.380) for $n > N_6$ that

$$t(G_{\bar{V}(n), \bar{N}(n)}) = C_8 + \frac{C_9}{4(C_3 + C_{13})} \ln(n+1) + \bar{\tau} \quad (5.382)$$

$$\leq \left(C_8 + \frac{C_9}{4(C_3 + C_{13})} + \bar{\tau} \right) \ln(n+1) \quad (5.383)$$

with $\bar{\tau}$ given in (5.242), (5.268), (5.273), (5.282), respectively.

Since for the first factor in (5.383) we have by (5.44), (5.135), (5.144) and (5.145) that

$$C_8 + \frac{C_9}{4(C_3 + C_{13})} + \bar{\tau} = \frac{16L}{B} + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + \frac{\sqrt{2\pi \mathcal{K}m}}{24\rho} + \bar{\tau}$$

(D_b, D_c given in (5.25)), it follows for (5.382) that

$$t(G_{\bar{V}(n), \bar{N}(n)}) \leq C_{16} \ln(n+1) \quad (5.384)$$

with

$$C_{16} := \frac{16L}{B} + \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} + \frac{\sqrt{2\pi \mathcal{K}m}}{24\rho} + \bar{\tau}$$

for any $n > N_6$.

So far, we made a choice on $\bar{N}(n)$ and $\bar{V}(n)$ (cf. (5.360), (5.371)) such that (5.351) for C_{14} given in (5.375) is satisfied for $n > \tilde{N}$ (cf. (5.374)), and which determines $\gamma(G_{\bar{V}(n), \bar{N}(n)})$ and gives an estimate for $t(G_{\bar{V}(n), \bar{N}(n)})$ (cf. (5.378) resp. (5.384)). To obtain the inequalities in Lemma 5.9, we now give a lower bound for the r.h.s. of (5.349), namely for

$$\beta \left((n+1)t(G_{\bar{V}(n), \bar{N}(n)}) \right) \quad (5.385)$$

and an upper bound for the l.h.s. of (5.350), namely for

$$2 \left(\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)})}{2} \right)^{n+1} + 8(n+1)\Pi(G_{\bar{V}(n), \bar{N}(n)}^c). \quad (5.386)$$

To estimate (5.385) we use the fact that $\beta(t)$ (cf. (5.5)) is non-increasing. This follows since for $t_1 < t_2$ the supremum in (5.5) for $\beta(t_2)$ is taken over $\mathcal{F}_{-\infty, 0} \times \mathcal{F}_{t_2, \infty} \subseteq \mathcal{F}_{-\infty, 0} \times \mathcal{F}_{t_1, \infty}$.

Let $n > N_6$. By (5.384) and since β is non-increasing we estimate (5.385) with

$$\beta((n+1)t(G_{\bar{V}(n), \bar{N}(n)})) \stackrel{(5.384)}{\geq} \beta(C_{16}(n+1)\ln(n+1)). \quad (5.387)$$

Since any root grows faster than the \ln -function there exists $N_7 \in \mathbb{N}$ such that for any $n > N_7$ it follows for the r.h.s. of (5.387) that

$$\beta(C_{16}(n+1)\ln(n+1)) \geq \beta((n+1)^{\frac{5}{4}}),$$

i.e. we have for (5.387) that

$$\beta((n+1)t(G_{\bar{V}(n), \bar{N}(n)})) \geq \beta((n+1)^{\frac{5}{4}}). \quad (5.388)$$

For (5.386) we obtain by (5.378) and (5.351) that for $n > \max\{\tilde{N}, N_5\}$ (cf. (5.374))

$$2 \left(\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)})}{2} \right)^{n+1} + 8(n+1)\Pi(G_{\bar{V}(n), \bar{N}(n)}^c) \quad (5.389)$$

$$\leq 2(1 - C_{15}(n+1)^{-\frac{1}{2}})^{n+1} + C_{14}(n+1)^{-5}. \quad (5.390)$$

Observe that

$$\ln(1 - C_{15}(n+1)^{-\frac{1}{2}}) \leq -C_{15}(n+1)^{-\frac{1}{2}},$$

so that for (5.390) we have that

$$2(1 - C_{15}(n+1)^{-\frac{1}{2}})^{n+1} + C_{14}(n+1)^{-5} \leq 2e^{-C_{15}(n+1)^{\frac{1}{2}}} + C_{14}(n+1)^{-5}, \quad (5.391)$$

and altogether for (5.389) by (5.390) and (5.391)

$$2 \left(\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)})}{2} \right)^{n+1} + 8(n+1)\Pi(G_{\bar{V}(n), \bar{N}(n)}^c) \leq 2e^{-C_{15}(n+1)^{\frac{1}{2}}} + C_{14}(n+1)^{-5}. \quad (5.392)$$

Choosing

$$i(n) = (n+1)^{\frac{5}{4}} \quad (5.393)$$

yields in (5.388) to

$$\beta((n+1)t(G_{\bar{V}(n), \bar{N}(n)})) \geq \beta(i(n)),$$

and in (5.392) to

$$2 \left(\frac{\gamma \left(G_{\bar{V}(n), \bar{N}(n)} \right)}{2} \right)^{n+1} + 8(n+1) \Pi \left(G_{\bar{V}(n), \bar{N}(n)}^c \right) \leq 2e^{-C_{15}i(n)^{\frac{2}{5}}} + C_{14}i(n)^{-4}.$$

Lemma 5.9 follows by choosing

$$A_1 = C_{15} \tag{5.394}$$

with C_{15} given in (5.379),

$$A_2 = C_{14} \tag{5.395}$$

with C_{14} given in (5.375) and

$$N = \max\{\tilde{N}, N_5, N_6, N_7\}. \tag{5.396}$$

□

Since $G_{\bar{V}(n), \bar{N}(n)}$ satisfies the conditions of the Overlap-Lemma 5.2 (see (5.318)), and Corollary 5.2 is about sets which satisfy the Overlap-Lemma 5.2, taking Corollary 5.2 and Lemma 5.9 together we obtain that for A_1, A_2 as chosen in (5.394) resp. (5.395), N as given in (5.396), $\bar{N}(n), \bar{V}(n), i(n)$ as defined in (5.360), (5.371) (5.393) respectively,

$$\begin{aligned} \beta(i(n)) &\stackrel{(5.349)}{<} \beta((n+1)t(G_{\bar{V}(n), \bar{N}(n)})) \\ &\stackrel{(5.342)}{<} 2 \left(\frac{\gamma \left(G_{\bar{V}(n), \bar{N}(n)} \right)}{2} \right)^{n+1} + 8(n+1) \Pi \left(G_{\bar{V}(n), \bar{N}(n)}^c \right) \\ &\stackrel{(5.350)}{<} 2 \exp(-A_1 i(n)^{\frac{2}{5}}) + A_2 i(n)^{-4} \end{aligned} \tag{5.397}$$

for all $n > N$. By this estimate for the β -coefficient (cf. (5.4)) of the process \mathcal{M}_t (cf. (5.7)) we finally can prove Proposition 5.1.

Proof of Proposition 5.1. Recall that $\mathbb{E}(|U(0)|^{2+\delta}) < \infty$ is true for any $\delta > 0$ (cf. Chapter 4). By the integral criterion we have that

$$\int_0^\infty \beta(t)^{\frac{\delta}{2+\delta}} dt < \infty \Leftrightarrow \sum_{j=0}^\infty \beta(j)^{\frac{\delta}{2+\delta}} < \infty, \delta > 0, \tag{5.398}$$

i.e. we obtain Proposition 5.1 as soon as we can show that there exists $\delta > 0$ such that

$$\sum_{j=0}^\infty \beta(j)^{\frac{\delta}{2+\delta}} < \infty.$$

By (5.397) there exist constants A_1, A_2 , a $N \in \mathbb{N}$ such that for any $n > N$ and $i(n) = (n+1)^{\frac{5}{4}}$

$$\beta(i(n)) < 2 \exp\left(-A_1 i(n)^{\frac{2}{5}}\right) + A_2 i(n)^{-4}, \quad (5.399)$$

and since $\beta(t)$ is non-decreasing, we have that for all $n \geq N+1$

$$\begin{aligned} \beta(\lfloor i(n) \rfloor + 1) &\stackrel{(5.399)}{\leq} \beta(i(n)) < 2 \exp\left(-A_1 i(n)^{\frac{2}{5}}\right) + A_2 i(n)^{-4} \\ &\leq 2 \exp\left(-A_1 \lfloor i(n) \rfloor^{\frac{2}{5}}\right) + A_2 \lfloor i(n) \rfloor^{-4}. \end{aligned} \quad (5.400)$$

Therefore, it is useful to write

$$\sum_{j=0}^{\infty} \beta(j)^{\frac{\delta}{2+\delta}} = \sum_{j=0}^{\lfloor i(N+1) \rfloor} \beta(j)^{\frac{\delta}{2+\delta}} + \sum_{j=\lfloor i(N+1) \rfloor + 1}^{\infty} \beta(j)^{\frac{\delta}{2+\delta}}. \quad (5.401)$$

Since the first sum on the r.h.s. in (5.401) is finite, we continue with the second sum in (5.401) and obtain by (5.400) that

$$\begin{aligned} \sum_{j=\lfloor i(N+1) \rfloor + 1}^{\infty} \beta(j)^{\frac{\delta}{2+\delta}} &< \sum_{j=\lfloor i(N+1) \rfloor}^{\infty} \left(2 \exp\left(-A_1 j^{\frac{2}{5}}\right) + A_2 j^{-4}\right)^{\frac{\delta}{2+\delta}} \\ &\leq \sum_{j=\lfloor i(N+1) \rfloor}^{\infty} \left(2 \exp\left(-A_1 j^{\frac{2}{5}}\right)\right)^{\frac{\delta}{2+\delta}} + \left(A_2 j^{-4}\right)^{\frac{\delta}{2+\delta}} \\ &= 2^{\frac{\delta}{2+\delta}} \sum_{j=\lfloor i(N+1) \rfloor}^{\infty} \left(\exp\left(-\frac{\delta A_1}{2+\delta} j^{\frac{2}{5}}\right)\right) + A_2^{\frac{\delta}{2+\delta}} \sum_{j=\lfloor i(N+1) \rfloor}^{\infty} j^{-\frac{4\delta}{2+\delta}}. \end{aligned} \quad (5.402)$$

Note that $A_1 > 0$ and $\frac{\delta}{2+\delta} > 0$, i.e. the first sum in (5.402) converges. The convergence of the second sum in (5.402) follows if

$$j^{-\frac{4\delta}{2+\delta}} \leq j^{-2},$$

which is satisfied for $\delta \geq 2$. Hence, we obtain by (5.401) and (5.402) that for any $\delta \geq 2$

$$\sum_{j=0}^{\infty} \beta(j)^{\frac{\delta}{2+\delta}} < \infty.$$

Proposition 5.1 follows immediately by (5.398). □

6 Proof: $D > 0$

In this chapter, we prove that

$$D = 2 \int_0^\infty \mathbb{E}(U(0)U(t))dt > 0. \quad (6.1)$$

Together with the proof that U_t is α -mixing with (3.5) (see Section 5.2), we then obtain our main result, since then we showed that our model satisfies all conditions of the fCLT (Theorem 3.1), which gives Theorem 2.1, our main result. Note that

$$2 \int_0^\infty \mathbb{E}(U(0)U(t))dt < \infty$$

follows by Theorem 3.1 from Proposition 5.1 (which is proved in Section 5.2).

The positivity of the diffusion constant (cf. (6.1)) follows as soon as we prove Condition (3.6) of Theorem 3.1, namely that

$$\sup_t \mathbb{E}(|R(t)|) \stackrel{(2.12)}{=} \sup_t \mathbb{E} \left(\left| \int_0^t U(s)ds \right| \right) = \infty \quad (6.2)$$

with $R(t)$ given in (2.12) and \mathbb{E} denotes the expectation w.r.t. the stationary measure of U_t given in (4.4). Since by the Markov inequality for any $C > 0$

$$\begin{aligned} \mathbb{E}(|R(t)|) &\geq C\mu \times \rho_{\frac{1}{2}}(|R(t)| > C) \\ &\stackrel{(2.12)}{=} C\mu \times \rho_{\frac{1}{2}} \left(\left| \int_0^t U(s)ds \right| > C \right), \end{aligned}$$

we may estimate the l.h.s. of (6.2) by

$$\sup_t \mathbb{E}(|R(t)|) \geq C \sup_t \mu \times \rho_{\frac{1}{2}} \left(\left| \int_0^t U(s)ds \right| > C \right). \quad (6.3)$$

Now assume we can show that there exists $\varepsilon > 0$ such that for any $C > 0$

$$\sup_t \mu \times \rho_{\frac{1}{2}} \left(\left| \int_0^t U(s)ds \right| > C \right) > \varepsilon,$$

then we obtain by (6.3) that

$$\sup_t \mathbb{E}(|R(t)|) \geq C\varepsilon.$$

Since C can be chosen arbitrarily large, (6.2) follows, which is Condition (3.6) of Theorem 3.1, and with that we obtain (6.1).

Hence, (6.1) follows as soon we can prove following proposition.

Proposition 6.1. There exists $\varepsilon > 0$ such that for any $C > 0$

$$\sup_t \mu \times \rho_{\frac{1}{2}} \left(\left| \int_0^t U(s) ds \right| > C \right) > \varepsilon. \quad (6.4)$$

Heuristically Proposition 6.1 says that $R_t = \{\int_0^t U(s) ds\}_{t \in \mathbb{R}^+}$ spreads unboundedly.

The idea of proving Proposition 6.1 is roughly the following. First, we add $Q(0)$ to $\int_0^t U(s) ds$, and we define

$$S(t) := \int_0^t U(s) ds + Q(0) \stackrel{(2.13)}{=} \int_0^t \sigma(s) V(s) ds + Q(0) \quad (6.5)$$

and, for reasons that become clear later, we define $S(t)$ with $\sigma(0) = 1$. Note that $S(t)$ is a random variable on $(\hat{\Omega}, \mathcal{F}, \mu)$ with $\hat{\Omega}$ given in (2.3) and μ given in (2.9), since for given $\sigma(0)$, $\{\sigma(t)\}_{t>0}$ is a process on $(\hat{\Omega}, \mathcal{F}, \mu)$. We first show that $S_t := \{S(t)\}_{t \in \mathbb{R}^+}$ spreads over \mathbb{R} . Since in this case no probability distribution exists, we observe $S(t)$ on a torus I_k , introducing $S_k(t)$. $S_k(t)$ is a function of $Q(t)$ and $j_k(t)$, where $j_k(t)$ is a new random variable we introduce to describe $S_k(t)$. Note that $S_k(t)$ depends on $Q(t)$, because by adding $Q(0)$ we linked $S(t)$ to the position of the molecule. Then, we use a Markov process which contains $Q(t)$, $j_k(t)$ from which we can make conclusions about the distribution of $S_{k,t} = \{S_k(t)\}_{t \in \mathbb{R}^+}$ for $t \rightarrow \infty$ and by that we show that S_t spreads unboundedly. Since $S(t)$ is given by (6.5), the spreading of $\int_0^t U(s) ds$ follows and we obtain Proposition 6.1.

We start now by observing $S(t)$ on a torus I_k , introducing by that $S_k(t)$. Let

$$I_k := (-2kL, 2kL] \text{ for } k = 1, 2, \dots \quad (6.6)$$

and consider the process

$$S_{k,t} := \{S_k(t)\}_{t \in \mathbb{R}^+} \quad (6.7)$$

with

$$S_k(t) := S(t) \bmod I_k, \quad (6.8)$$

where

$$x \bmod (a, b] := x - (b - a) \left\lfloor \frac{x - a}{b - a} \right\rfloor \quad (6.9)$$

with

$$\lfloor y \rfloor := \max\{k \in \mathbb{Z} : k \leq y\}. \quad (6.10)$$

Note for later use that for $z \in \mathbb{Z}$

$$x, x' \in (zb - (z - 1)a, (z + 1)b - za] \Rightarrow \left\lfloor \frac{x - a}{b - a} \right\rfloor = \left\lfloor \frac{x' - a}{b - a} \right\rfloor. \quad (6.11)$$

We now prove that for any $k \in \mathbb{N}$ $S_{k,t}$ uniformly spreads over the torus as t approaches infinity. Therefore, it is useful to encode $S_k(t)$ in a more appropriate manner. Separate the interval I_k into $2k$ intervals and numbering them, such that

$$(-(2k - 1)L + 2(j - 1)L, -(2k - 1)L + 2jL) \quad (6.12)$$

is the j -th interval with $j \in \{1, 2, \dots, 2k - 1\}$, where

$$(-2kL, -2kL + L) \cup (2kL - L, 2kL) \quad (6.13)$$

is the interval with number 0. Denote by

$$j_k(t) \in \{0, 1, 2, \dots, 2k - 1\} =: \mathcal{J}_k \quad (6.14)$$

the number of the interval in which $S_k(t)$ is at time t whereby $j_k(t)$ changes its value as soon as

$$S_k(t) \in \bigcup_{j \in \mathbb{Z}} \{-(2k - 1)L + 2(j - 1)L\} \cap I_k, \quad (6.15)$$

such that $S_k(t) = -(2k - 1)L + 2(j - 1)L$ and $j_k(t) = j$ means that S_k goes through $-(2k - 1)L + 2(j - 1)L$ from left to right, and $S_k(t) = -(2k - 1)L + 2(j - 1)L$ and $j_k(t) = j - 1$ means that S_k goes through $-(2k - 1)L + 2(j - 1)L$ from right to left. Note that by definition of $S_k(t)$ (cf. (6.8)) and $S(t)$ (cf. (6.5)) we have that $j_k(0) = k$, since $S_k(0) = Q(0) \in [-L, L]$.

We now show that $S_k(t)$ is determined by $Q(t)$ and $j_k(t)$, i.e. that $S_k(t)$ is a function of $Q(t)$ and $j_k(t)$. This circumstance is based on the facts that $S_k(t)$ is defined with $\sigma(0) = 1$ and that the modulus I_k is such that $j_k(t)$ determines the value of $\sigma(t)$. With that, the values of $Q(t)$ and $j_k(t)$ give a good enough restriction for the possible values for $S_k(t)$ such that $S_k(t)$ is fully determined.¹

¹If one defined $S_{k,t}$ such that $\sigma(0) = -1$, $S_k(t)$ would not be fully determined by $Q(t)$ and $j_k(t)$ (also $Q(0)$ is necessary). Since in addition $j_k(t)$ would not determine $\sigma(t)$, the methods we use in the presented proof cannot be transferred to this case.

For the proof we use various assertions which follow by elementary algebra. Let us give a short overview about the content of these assertions. First, we show by Assertion 6.1, Assertion 6.2 and Assertion 6.3 how $S(t)$ resp. $S_k(t)$ depends on $\sigma(t)$, whereas Assertion 6.4 is about the dependence between $S_k(t)$ and certain values of $Q(t)$. Assertion 6.5 and Assertion 6.6 are about $j_k(t)$. The first is about the relation to $\sigma(t)$, the latter shows how $j_k(t)$ changes its value dependent on $Q(t)$. By these assertions it becomes clear that $j_k(t)$ changes its value iff $\sigma(t)$ changes its value, namely when the molecule is reflected at one of the walls, and moreover we show that the value of $\sigma(t)$ can be derived by the value of $j_k(t)$, such that in Lemma 6.1 we can prove that $S_k(t)$ is fully determined by $Q(t)$ and $j_k(t)$.

Before we show how $S_k(t)$ (cf. (6.8)) depends on $\sigma(t)$, we have to show how $S(t)$ (cf. (6.5)) depends on $\sigma(t)$.

Assertion 6.1. Consider $S(t)$ as defined in (6.5). If for some $t > 0$

$$\sigma(0) = 1 \text{ and } \sigma(t) = 1 \Rightarrow S(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 1)L, (4i + 1)L] \quad (6.16)$$

and if

$$\sigma(0) = 1 \text{ and } \sigma(t) = -1 \Rightarrow S(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 3)L, (4i - 1)L]. \quad (6.17)$$

Proof of Assertion 6.1. Let $\sigma(0) = 1$. Since by definition $\sigma(t)$ changes its value, when $Q(t) \in \{-L, L\}$, we can follow from $\sigma(t) = 1$ that the molecule is reflected at the walls of Λ an even number of times during the time interval $[0, t]$, and from $\sigma(t) = -1$ that the molecule is reflected during $[0, t]$ an odd number of times.

Before we prove (6.16) and (6.17), we express $S(t)$ in a more appropriate manner. Consider the molecule is reflected during $[0, t]$ $n_t \geq 1$ times and denote by τ_i , $i \in \{1, \dots, n_t\}$ the time of the i -th reflection, i.e.

$$Q(\tau_i) \in \{-L, L\}, i \in \{1, \dots, n_t\}. \quad (6.18)$$

Then, we can write

$$\begin{aligned} S(t) &\stackrel{(6.5)}{=} Q(0) + \int_0^t \sigma(s)V(s)ds \\ &= Q(0) + \int_0^{\tau_1} V(s)ds + \sum_{i=1}^{n_t-1} (-1)^i \int_{\tau_i}^{\tau_{i+1}} V(s)ds + (-1)^{n_t} \int_{\tau_{n_t}}^t V(s)ds. \end{aligned} \quad (6.19)$$

Since

$$Q(0) + \int_0^{\tau_1} V(s)ds = Q(\tau_1), \quad (6.20)$$

$$\int_{\tau_i}^{\tau_{i+1}} V(s)ds = Q(\tau_{i+1}) - Q(\tau_i) \quad (6.21)$$

and

$$\int_{\tau_{n_t}}^t V(s)ds = Q(t) - Q(\tau_{n_t}), \quad (6.22)$$

we obtain for (6.19) that

$$\begin{aligned} S(t) &= Q(0) + \int_0^{\tau_1} V(s)ds + \sum_{i=1}^{n_t-1} (-1)^i \int_{\tau_i}^{\tau_{i+1}} V(s)ds + (-1)^{n_t} \int_{\tau_{n_t}}^t V(s)ds \\ &\stackrel{(6.20),(6.21),(6.22)}{=} Q(\tau_1) + \sum_{i=1}^{n_t-1} (-1)^i (Q(\tau_{i+1}) - Q(\tau_i)) + (-1)^{n_t} (Q(t) - Q(\tau_{n_t})) \\ &= \sum_{i=1}^{n_t} (-1)^{i+1} 2Q(\tau_i) + (-1)^{n_t} Q(t). \end{aligned} \quad (6.23)$$

Now consider $\sigma(t) = 1$, i.e. the molecule is reflected $n_t \in 2\mathbb{N}$ times during $[0, t]$. Then, from (6.23) it follows that

$$S(t) = \sum_{i=1}^{n_t} (-1)^{i+1} 2Q(\tau_i) + Q(t). \quad (6.24)$$

With (6.18) it follows for the sum in (6.24) that

$$\sum_{i=1}^{n_t} (-1)^{i+1} 2Q(\tau_i) \in \bigcup_{i=1}^{n_t+1} \{-2n_t L + 4L(i-1)\}. \quad (6.25)$$

Since $Q(t) \in [-L, L]$, we have for (6.24) with (6.25) that

$$S(t) \in \bigcup_{i=1}^{n_t+1} [-2n_t L + 4L(i-1) - L, -2n_t L + 4L(i-1) + L]. \quad (6.26)$$

Since for any $n_t \in 2\mathbb{N}$ for the r.h.s. of (6.26) we have that

$$\begin{aligned} &\bigcup_{i=1}^{n_t+1} [-2n_t L + 4L(i-1) - L, -2n_t L + 4L(i-1) + L] \\ &= \bigcup_{i=1}^{n_t+1} [(-2n_t + 4(i-1) - 1)L, (-2n_t + 4(i-1) + 1)L] \end{aligned}$$

$$\subset \bigcup_{i \in \mathbb{Z}} [(4i - 1)L, (4i + 1)L], \quad (6.27)$$

it follows by (6.26) and (6.27) that

$$S(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 1)L, (4i + 1)L] \quad (6.28)$$

Consider now $n_t = 0$. Then,

$$S(t) \stackrel{(6.5)}{=} Q(t) \in [-L, L] \subset \bigcup_{i \in \mathbb{Z}} [(4i - 1)L, (4i + 1)L]. \quad (6.29)$$

(6.16) follows by (6.28) and (6.29).

Since (6.17) can be proven analogously, Assertion 6.1 follows. □

By Assertion 6.1 we can make a statement about how $S_k(t)$ (cf. (6.8)) depends on $\sigma(t)$.

Assertion 6.2. Let $k \in \mathbb{N}$. Consider $S_k(t)$ as given in (6.8). Then, if for some $t > 0$

$$\sigma(0) = 1 \text{ and } \sigma(t) = 1 \Rightarrow S_k(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 1)L, (4i + 1)L] \cap I_k \quad (6.30)$$

and if

$$\sigma(0) = 1 \text{ and } \sigma(t) = -1 \Rightarrow S_k(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 3)L, (4i - 1)L] \cap I_k. \quad (6.31)$$

Proof of Assertion 6.2. Consider $\sigma(0) = 1$ and $\sigma(t) = 1$. Then, by Assertion 6.1

$$S(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 1)L, (4i + 1)L]. \quad (6.32)$$

To prove (6.30) we have to show that the modulus I_k just restrict the range of values given by (6.32), i.e. such that with (6.32)

$$S(t) \bmod I_k = S_k(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 1)L, (4i + 1)L] \cap I_k.$$

To begin we define

$$\begin{aligned} \text{Mod}_k : \mathbb{R} &\rightarrow I_k, \\ x &\mapsto x \bmod I_k \end{aligned} \quad (6.33)$$

with I_k given in (6.6). We first show that for any boundary point of the subintervals in (6.32), i.e. for any $i \in \mathbb{Z} \exists l_1, l_2 \in \mathbb{Z}$ such that

$$\text{Mod}_k((4i - 1)L) = (4l_1 - 1)L, \quad (6.34)$$

$$\text{Mod}_k((4i + 1)L) = (4l_2 + 1)L. \quad (6.35)$$

Let $i \in \mathbb{Z}$. For the l.h.s. of (6.34) we have that

$$\begin{aligned} \text{Mod}_k((4i - 1)L) &\stackrel{(6.33)}{=} (4i - 1)L \bmod I_k \\ &\stackrel{(6.6), (6.9)}{=} (4i - 1)L - 4kL \left\lfloor \frac{(4i - 1)L - (-2kL)}{4kL} \right\rfloor. \end{aligned} \quad (6.36)$$

Since by the definition of $\lfloor \cdot \rfloor$ (cf. (6.10)) $\exists y_1 \in \mathbb{Z}$ such that

$$y_1 = \left\lfloor \frac{(4i - 1)L - (-2kL)}{4kL} \right\rfloor, \quad (6.37)$$

we obtain for (6.36) that

$$\begin{aligned} \text{Mod}_k((4i - 1)L) &= 4iL - L - 4kLy_1 \\ &= (4(i - ky_1) - 1)L \\ &= (4l_1 - 1)L. \end{aligned} \quad (6.38)$$

with

$$l_1 := i - ky_1 \in \mathbb{Z}. \quad (6.39)$$

For the l.h.s. of (6.35) we have that

$$\begin{aligned} \text{Mod}_k((4i + 1)L) &\stackrel{(6.33)}{=} (4i + 1)L \bmod I_k \\ &\stackrel{(6.6), (6.9)}{=} (4i + 1)L - 4kL \left\lfloor \frac{(4i + 1)L - (-2kL)}{4kL} \right\rfloor \\ &= (4i + 1)L - 4kLy_2 \end{aligned} \quad (6.40)$$

$$= (4l_2 + 1)L \quad (6.41)$$

with

$$l_2 := i - ky_2 \in \mathbb{Z}. \quad (6.42)$$

Since (6.32) there is a $i \in \mathbb{N}$ such that

$$S(t) = s \in [(4i - 1)L, (4i + 1)L]. \quad (6.43)$$

Having (6.11) in mind, we now distinguish if there is a $z \in \mathbb{Z}$ such that

$$[(4i-1)L, (4i+1)L] \subseteq ((2z-1)2kL, (2z+1)2kL) := I_{k,z} \quad (6.44)$$

or if there is no such z , i.e.

$$\nexists z \in \mathbb{Z} : [(4i-1)L, (4i+1)L] \subseteq I_{k,z}. \quad (6.45)$$

If (6.44), then by (6.11) we have that

$$y_1 = y_2$$

with y_1 given in (6.37) and y_2 given in (6.40) and with that

$$l_1 = l_2 \quad (6.46)$$

with l_1 given in (6.39) and l_2 given in (6.42). With (6.43) it follows by the monotonicity of Mod_k (cf. (6.33)) that

$$(4l_1 - 1)L \stackrel{(6.38)}{=} Mod_k((4i-1)L) \leq Mod_k(s) \leq Mod_k((4i+1)L) \stackrel{(6.41),(6.46)}{=} (4l_1 + 1)L.$$

i.e. with (6.43)

$$S_k(t) \stackrel{(6.8),(6.33)}{=} Mod_k(s) \in [(4l_1 - 1)L, (4l_1 + 1)L] \subset \bigcup_{i \in \mathbb{Z}} [(4i-1)L, (4i+1)L] \cap I_k.$$

Now if (6.45), then by definition of $I_{k,z}$ (cf. (6.44)) there is a $z \in \mathbb{Z}$ such that

$$[(4i-1)L, 4iL] \in I_{k,z} \text{ and } [4iL, (4i+1)L] \in I_{k,z+1}.$$

We have then that if

$$\begin{aligned} s \in [(4i-1)L, 4iL] \Rightarrow \\ (4l_1 - 1)L \stackrel{(6.38)}{=} Mod_k((4i-1)L) \leq Mod_k(s) \leq (4l_1 - 1)L + L \end{aligned}$$

and if

$$s \in [4iL, (4i+1)L] \Rightarrow (4l_2 + 1)L - L < Mod_k(s) \leq Mod_k((4i+1)L) \stackrel{(6.41)}{=} (4l_2 + 1)L,$$

i.e. with (6.43) we have that

$$\begin{aligned} S_k(t) \stackrel{(6.8),(6.33)}{=} Mod_k(s) \in [(4l_1 - 1)L, 4l_1L] \cup [4l_2L, (4l_2 + 1)L] \\ \subset \bigcup_{i \in \mathbb{Z}} [(4i-1)L, (4i+1)L] \cap I_k. \end{aligned}$$

Since (6.31) can be proven analogously, Assertion 6.2 follows. □

By Assertion 6.2 following assertion follows immediately.

Assertion 6.3. Let $k \in \mathbb{N}$. Consider $S_k(t)$ as given in (6.8). Then, if for some $t > 0$

$$\sigma(0) = 1 \text{ and } S_k(t) \in \bigcup_{i \in \mathbb{Z}} ((4i - 1)L, (4i + 1)L) \cap I_k \Rightarrow \sigma(t) = 1 \quad (6.47)$$

and if

$$\sigma(0) = 1 \text{ and } S_k(t) \in \bigcup_{i \in \mathbb{Z}} ((4i - 3)L, (4i - 1)L) \cap I_k \Rightarrow \sigma(t) = -1.$$

Proof of Assertion 6.3. We show (6.47). Consider $\sigma(0) = 1$. Then, (6.47) follows as soon as we prove that if

$$\sigma(t) \neq 1 \Rightarrow S_k(t) \notin \bigcup_{i \in \mathbb{Z}} ((4i - 1)L, (4i + 1)L) \cap I_k. \quad (6.48)$$

The l.h.s. of (6.48) is equivalent to $\sigma(t) = -1$ and by Assertion 6.2 we have that

$$\sigma(t) = -1 \Rightarrow S_k(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 3)L, (4i - 1)L] \cap I_k. \quad (6.49)$$

Since

$$I_k \setminus \left(\bigcup_{i \in \mathbb{Z}} [(4i - 3)L, (4i - 1)L] \cap I_k \right) = \bigcup_{i \in \mathbb{Z}} ((4i - 1)L, (4i + 1)L) \cap I_k$$

for the r.h.s. of (6.49) it follows that

$$S_k(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 3)L, (4i - 1)L] \cap I_k \Leftrightarrow S_k(t) \notin \bigcup_{i \in \mathbb{Z}} ((4i - 1)L, (4i + 1)L) \cap I_k, \quad (6.50)$$

and all in all (6.48) follows since we have for the l.h.s. of (6.48) that

$$\begin{aligned} \sigma(t) \neq 1 &\Leftrightarrow \sigma(t) = -1 \\ &\stackrel{(6.49)}{\Rightarrow} S_k(t) \in \bigcup_{i \in \mathbb{Z}} [(4i - 3)L, (4i - 1)L] \cap I_k \end{aligned}$$

$$\stackrel{(6.50)}{\Leftrightarrow} S_k(t) \notin \bigcup_{i \in \mathbb{Z}} ((4i-1)L, (4i+1)L) \cap I_k.$$

(6.47) follows by similar arguments but using (6.30) of Assertion 6.2. \square

It turns out, if $Q(t)$ is given, the set of possible values of $S_k(t)$ differ dependent on the value of $j_k(t)$ except if $Q(t) \in \{-L, 0, L\}$. In the latter case the set of possible values for $S_k(t)$ are the same no matter which value $j_k(t)$ is. We can prove the following assertion.

Assertion 6.4. Let $k \in \mathbb{N}$. Consider $S_k(t)$ as defined in (6.8). Then, for $t \geq 0$

$$Q(t) = 0 \Leftrightarrow S_k(t) \in \bigcup_{i \in \mathbb{Z}} \{2iL\} \cap I_k, \quad (6.51)$$

and

$$Q(t) \in L \Leftrightarrow S_k(t) \in \bigcup_{i \in \mathbb{Z}} \{(4i+1)L\} \cap I_k, \quad (6.52)$$

and

$$Q(t) \in -L \Leftrightarrow S_k(t) \in \bigcup_{i \in \mathbb{Z}} \{(4i-1)L\} \cap I_k, \quad (6.53)$$

Proof of Assertion 6.4. We show (6.51). First, we handle “ \Rightarrow ”. Let

$$Q(t) = 0. \quad (6.54)$$

Consider the molecule is reflected $n_t \geq 1$ times during $[0, t]$ and denote by τ_i the time of the i -th reflection, i.e. $Q(\tau_i) \in \{-L, L\}$, $i \in \{1, \dots, n_t\}$. Hence, we can write $S(t)$ as given in (6.23) and with (6.54) it follows that

$$S(t) = \sum_{i=1}^{n_t} (-1)^{i+1} 2Q(\tau_i). \quad (6.55)$$

Since for any $i \in \{1, \dots, n_t\}$

$$(-1)^{i+1} 2Q(\tau_i) \in \{-2L, 2L\},$$

we have for (6.55) that

$$S(t) = \sum_{i=1}^{n_t} (-1)^{i+1} 2Q(\tau_i) \in \bigcup_{i=0}^{n_t} \{-n_t 2L + 4Li\}. \quad (6.56)$$

Now consider $n_t = 0$, i.e. the molecule hasn't been reflected during $[0, t]$. Then,

$$S(t) \stackrel{(6.5)}{=} Q(t) \stackrel{(6.54)}{=} 0. \quad (6.57)$$

Altogether we obtain with (6.56) and (6.57) that

$$\begin{aligned} Q(t) = 0 \Rightarrow S(t) &\in \bigcup_{n_t=0}^{\infty} \bigcup_{i=0}^{n_t} \{-2n_t L + 4Li\} \\ &= \bigcup_{i \in \mathbb{Z}} \{2iL\}. \end{aligned} \quad (6.58)$$

To prove “ \Rightarrow ” of (6.51), we have to show that the modulus restrict the range of values given by (6.58) in an appropriate way, i.e. such that if

$$S(t) \in \bigcup_{i \in \mathbb{Z}} \{2iL\} \Rightarrow S_k(t) \in \bigcup_{i \in \mathbb{Z}} \{2iL\} \cap I_k. \quad (6.59)$$

Consider

$$S(t) = 2iL. \quad (6.60)$$

If $2iL \in I_k$ then

$$\text{Mod}_k(2iL) \stackrel{(6.9)}{=} 2iL. \quad (6.61)$$

With

$$S_k(t) \stackrel{(6.8)}{=} S(t) \bmod I_k \stackrel{(6.33), (6.60)}{=} \text{Mod}_k(2iL) \stackrel{(6.61)}{=} 2iL \in I_k$$

the r.h.s. of (6.59) follows.

If $2iL \notin I_k$ we have that

$$\text{Mod}_k(2Li) \stackrel{(6.33)}{=} 2Li \bmod I_k \stackrel{(6.9)}{=} 2iL - 4kL \left\lfloor \frac{2iL + 2kL}{4kL} \right\rfloor.$$

Since $\lfloor \cdot \rfloor \in \mathbb{Z}$ by definition (cf. (6.10)), there is a $y \in \mathbb{Z}$ such that

$$\text{Mod}_k(2Li) = 2iL - 4kLy = 2L(i - 2ky) \in I_k, i - 2ky \in \mathbb{Z} \quad (6.62)$$

By (6.62) we obtain that

$$S_k(t) \stackrel{(6.8)}{=} S(t) \bmod I_k \stackrel{(6.33), (6.60)}{=} \text{Mod}_k(2iL) \in \bigcup_{i \in \mathbb{Z}} \{2iL\} \cap I_k,$$

and the r.h.s. of (6.59) follows.

Altogether, by (6.58) and (6.59) we have shown “ \Rightarrow ” of (6.51).

Now we show “ \Leftarrow ” of (6.51).

Consider

$$S_k(t) \in \bigcup_{i \in \mathbb{Z}} \{2iL\} \cap I_k.$$

We have to show that then $Q(t) = 0$ follows. Since for some appropriate constant $y \in \mathbb{Z}$ we have that

$$S_k(t) \stackrel{(6.8)(6.9)}{=} S(t) - 4kL \left\lfloor \frac{S(t) + 2kL}{4kL} \right\rfloor = S(t) - 4kLy,$$

we obtain that if

$$S_k(t) \in \bigcup_{i \in \mathbb{Z}} \{2iL\} \cap I_k \Rightarrow S(t) \in \bigcup_{i \in \mathbb{Z}} \{2iL\}. \quad (6.63)$$

Assume the molecule collides $n_t \geq 1$ times with $-L$ or L during $[0, t]$, then we can use (6.23) and write

$$S(t) = \sum_{i=1}^{n_t} (-1)^{i+1} 2Q(\tau_i) + (-1)^{n_t} Q(t) \quad (6.64)$$

Since for any $i \in \{1, \dots, n_t\}$

$$(-1)^{i+1} 2Q(\tau_i) \in \{-2L, 2L\},$$

we have for the sum in (6.64) that

$$\sum_{i=1}^{n_t} (-1)^{i+1} 2Q(\tau_i) \in \bigcup_{i=0}^{n_t} \{-2n_tL + 4Li\}.$$

Let j such that

$$\sum_{i=1}^{n_t} (-1)^{i+1} 2Q(\tau_i) = -2n_tL + 4jL. \quad (6.65)$$

Plugging (6.65) into (6.64) we obtain that

$$\begin{aligned} S(t) &= \sum_{i=1}^{n_t} (-1)^{i+1} 2Q(\tau_i) + (-1)^{n_t} Q(t) \\ &\stackrel{(6.65)}{=} -2n_tL + 4jL + (-1)^{n_t} Q(t). \end{aligned} \quad (6.66)$$

In addition by the r.h.s. of (6.63) we know that there is a $m \in \mathbb{Z}$ such that

$$S(t) = 2mL. \quad (6.67)$$

Since $Q(t)$ in (6.66) and m in (6.67) have to be such that

$$\begin{aligned} -2n_tL + 4jL + (-1)^{n_t}Q(t) &= 2mL \\ \Leftrightarrow (-1)^{n_t}Q(t) &= 2mL + 2n_tL - 4jL \\ \Leftrightarrow (-1)^{n_t}Q(t) &= 2L(m + n_t - 4j). \end{aligned} \quad (6.68)$$

Since $m + n_t - 4j \in \mathbb{Z}$ and $Q(t) \in [-L, L]$ it follows from (6.68) that $m + n_t - 4j = 0$ and

$$Q(t) = 0. \quad (6.69)$$

Now consider $n_t = 0$, i.e. the molecule hasn't been reflected during $[0, t]$. Then,

$$S(t) \stackrel{(6.5)}{=} Q(t). \quad (6.70)$$

By the r.h.s. of (6.63) there exists a $m \in \mathbb{Z}$ such that

$$S(t) = 2mL,$$

and with (6.70) it follows that

$$2mL = Q(t) \Leftrightarrow m = 0, Q(t) = 0. \quad (6.71)$$

All in all we obtain by (6.69) and (6.71) that

$$S_k(t) \in \bigcup_{i \in \mathbb{Z}} \{2iL\} \cap I_k \Rightarrow Q(t) = 0,$$

which gives (6.51).

Since (6.52) and (6.53) follow by the arguments we used to prove (6.51), Assertion 6.4 follows. □

The following assertion, which can be proved by Assertion 6.3 and Assertion 6.4, is about the relation of $j_k(t)$ and $\sigma(t)$.

Assertion 6.5. Let $k \in \mathbb{N}$ and $\sigma(0) = 1$. Consider $t > 0$ and $j_k(t) = j \in \mathcal{J}_k$ (cf. (6.14)). Denote by τ_e the last time before time t , when the molecule was at $-L$ or L . Then, if

$\tau_e \neq t$, i.e. $\tau_e < t$, and

$$j \in 2\mathbb{Z} + k \Rightarrow \sigma(t') = 1, \tau_e \leq t' \leq t \quad (6.72)$$

and if

$$j \in 2\mathbb{Z} + k + 1 \Rightarrow \sigma(t') = -1, \tau_e \leq t' \leq t. \quad (6.73)$$

Note that Assertion 6.5 says that $j_k(t)$ and $\sigma(t)$ change their values at the same time namely when $Q(t) \in \{-L, L\}$.

Proof of Assertion 6.5. Let $\sigma(0) = 1$ and $\tau_e < t$. Consider

$$j_k(t) = j \in 2\mathbb{Z} + k.$$

Then, by definition of $j_k(t)$ with (6.12), it follows that

$$S_k(t) \in \bigcup_{j \in 2\mathbb{Z} + k} [-(2k-1)L + 2(j-1)L, -(2k-1)L + 2jL] \cap I_k, \quad (6.74)$$

and by definition of τ_e it holds that

$$Q(t) \notin \{-L, L\}.$$

By Assertion 6.4 we have that

$$Q(t) \notin \{-L, L\} \Leftrightarrow S_k(t) \notin \bigcup_{i \in \mathbb{Z}} \{2iL\} \cap I_k$$

which yields with (6.74) to

$$S_k(t) \in \bigcup_{j \in 2\mathbb{Z} + k} (-(2k-1)L + 2(j-1)L, -(2k-1)L + 2jL) \cap I_k. \quad (6.75)$$

Since for the r.h.s. of (6.75) we have that

$$\bigcup_{j \in 2\mathbb{Z} + k} (-(2k-1)L + 2(j-1)L, -(2k-1)L + 2jL) \cap I_k = \bigcup_{i \in \mathbb{Z}} ((4i-1)L, (4i+1)L) \cap I_k \quad (6.76)$$

by Assertion 6.3 we can follow from (6.75) and (6.76) that

$$\sigma(t) = 1.$$

Since $\sigma(t)$ changes its value iff the molecule is at L or $-L$, we have that $\sigma(\tau_e) = 1$, and (6.72) follows.

Since (6.73) follows by similar reasoning, we obtain Assertion 6.5. □

Now we show how $j_k(t)$ changes its value dependent on $Q(t)$.

Assertion 6.6. Let $k \in \mathbb{N}$. Consider $j_k(t)$ as defined in (6.14) and underneath. Denote by τ_e the last time before time t , when the molecule was at $-L$ or L , i.e. $Q(\tau_e) \in \{-L, L\}$ and by τ_{e-} the time right before τ_e . Then, if

$$j_k(t) = j \Rightarrow j_k(t') = j, \tau_e \leq t' \leq t \text{ and } j_k(\tau_{e-}) \neq j.$$

Proof of Assertion 6.6. Since by definition, $j_k(t)$ changes its value if and only if

$$S_k(t) \in \bigcup_{j \in \mathbb{Z}} \{-(2k-1)L + 2(j-1)L\} \cap I_k$$

(cf. (6.15)) and since with

$$\bigcup_{j \in \mathbb{Z}} \{-(2k-1)L + 2(j-1)L\} \cap I_k = \left(\bigcup_{i \in \mathbb{Z}} \{(4i-1)L\} \cup \bigcup_{i \in \mathbb{Z}} \{(4i+1)L\} \right) \cap I_k$$

we obtain by Assertion 6.4 that

$$S_k(t) \in \bigcup_{j \in \mathbb{Z}} \{-(2k-1)L + 2(j-1)L\} \cap I_k \Leftrightarrow Q(t) \in \{-L, L\},$$

and Assertion 6.6 follows. □

Finally, by Assertion 6.4, Assertion 6.5 and Assertion 6.6 we can prove that $S_k(t)$ (cf. (6.8)) is determined by $Q(t)$ and $j_k(t)$, i.e. $S_k(t)$ is a function of $Q(t), j_k(t)$.

Lemma 6.1. Let $k \in \mathbb{N}$. Consider $\sigma(0) = 1$. For any $t \geq 0$, $S_k(t)$ (cf. (6.8)) is determined by $Q(t)$ and $j_k(t)$ (cf. (6.14)) with

$$\begin{aligned} f : [-L, L] \times \mathcal{J}_k &\rightarrow I_k, \\ (Q(t), j_k(t)) &\mapsto S_k(t) \end{aligned}$$

where

$$S_k(t) = \begin{cases} Q(t) + 2L(j_k(t) - k) & , \text{ if } j_k(t) \in (2\mathbb{Z} + k) \setminus \{0\} \\ -Q(t) + 2L(j_k(t) - k) & , \text{ if } j_k(t) \in (2\mathbb{Z} + k + 1) \setminus \{0\} . \\ Q(t) - 2kL & , \text{ if } j_k(t) = 0 \in 2\mathbb{Z} + k, Q(t) \in [0, L] \\ Q(t) + 2kL & , \text{ if } j_k(t) = 0 \in 2\mathbb{Z} + k, Q(t) \in [-L, 0) \\ -Q(t) + 2kL & , \text{ if } j_k(t) = 0 \in 2\mathbb{Z} + k + 1, Q(t) \in [0, L] \\ -Q(t) - 2kL & , \text{ if } j_k(t) = 0 \in 2\mathbb{Z} + k + 1, Q(t) \in [-L, 0) \end{cases} \quad (6.77)$$

Proof of Lemma 6.1. Consider $\sigma(0) = 1$ and $j_k(t) = j \in \mathcal{J}_k \setminus \{0\}$. Then, by definition of $j_k(t)$ (cf. (6.14)) with (6.12) we have that

$$j_k(t) = j \Rightarrow S_k(t) \in [-(2k - 1)L + 2(j - 1)L, -(2k - 1)L + 2jL]. \quad (6.78)$$

Denote by τ_e the last time at which the molecule was reflected at one of the walls before t , i.e. $Q(\tau_e) = L$ or $Q(\tau_e) = -L$. Assume that

$$\tau_e \neq t$$

i.e.

$$\tau_e < t \quad (6.79)$$

Consider

$$Q(\tau_e) = L. \quad (6.80)$$

Then, by Assertion 6.4

$$S_k(\tau_e) \in \bigcup_{i \in \mathbb{Z}} \{(4i + 1)L\} \cap I_k, \quad (6.81)$$

and by Assertion 6.6

$$j_k(\tau_e) = j. \quad (6.82)$$

Consider $j \in 2\mathbb{Z} + k$. With (6.82) we have by (6.78) and (6.81) that

$$\begin{aligned} S_k(\tau_e) &\in [-(2k - 1)L + 2(j - 1)L, -(2k - 1)L + 2jL] \cap \bigcup_{i \in \mathbb{Z}} \{(4i + 1)L\} \cap I_k \\ &= \{-(2k - 1)L + 2jL\} \\ &= \{L + 2L(j - k)\}. \end{aligned} \quad (6.83)$$

Further, by definition of τ_e and Assertion 6.5 we have that $\sigma(t') = 1$ for $\tau_e \leq t' \leq t$. Since

then

$$S_k(t) \stackrel{(6.8)}{=} S_k(\tau_e) + \int_{\tau_e}^t \sigma(s)V(s)ds = S_k(\tau_e) + \int_{\tau_e}^t V(s)ds, \quad (6.84)$$

we obtain with

$$Q(t) = Q(\tau_e) + \int_{\tau_e}^t V(s)ds, \quad (6.85)$$

that

$$\begin{aligned} S_k(t) &\stackrel{(6.84)}{=} S_k(\tau_e) + \int_{\tau_e}^t V(s)ds \\ &\stackrel{(6.83)}{=} L + 2L(j - k) + \int_{\tau_e}^t V(s)ds \\ &\stackrel{(6.80)}{=} Q(\tau_e) + \int_{\tau_e}^t V(s)ds + 2L(j - k) \\ &\stackrel{(6.85)}{=} Q(t) + 2L(j - k), \end{aligned}$$

which gives the first line of (6.77).

If $j \in 2\mathbb{Z} + k + 1$ by Assertion 6.4 and (6.78) it follows that

$$\begin{aligned} S_k(\tau_e) &\in [-(2k - 1)L + 2(j - 1)L, -(2k - 1)L + 2jL] \cap \bigcup_{i \in \mathbb{Z}} \{(4i + 1)L\} \cap I_k \\ &= \{-(2k - 1)L + 2(j - 1)L\} \\ &= \{-L + 2L(j - k)\}. \end{aligned} \quad (6.86)$$

By Assertion 6.5 we have that $\sigma(t') = -1$ for $\tau_e \leq t' \leq t$. By

$$S_k(t) = S_k(\tau_e) + \int_{\tau_e}^t \sigma(s)V(s)ds = S_k(\tau_e) - \int_{\tau_e}^t V(s)ds \quad (6.87)$$

and (6.85) we obtain that

$$\begin{aligned} S_k(t) &\stackrel{(6.87)}{=} S_k(\tau_e) - \int_{\tau_e}^t V(s)ds \\ &\stackrel{(6.86)}{=} -L + 2L(j - k) - \int_{\tau_e}^t V(s)ds \\ &\stackrel{(6.85)}{=} -Q(t) + 2L(j - k), \end{aligned}$$

which gives the second line of (6.77).

Using the same method, (6.77) follows for $j = 0$.

If $Q(\tau_e) = -L$ we obtain (6.77) by the same arguments.

We considered in (6.79) that $\tau_e < t$. Now assume that

$$\tau_e = t. \quad (6.88)$$

Consider

$$Q(\tau_e) = L. \quad (6.89)$$

If $j \in 2\mathbb{Z} + k \setminus \{0\}$ we have by (6.78) and Assertion 6.4 that

$$\begin{aligned} S_k(t) &= S_k(\tau_e) \in [-(2k-1)L + 2(j-1)L, -(2k-1)L + 2jL] \cap \bigcup_{i \in \mathbb{Z}} \{(4i+1)L\} \cap I_k \\ &= \{-(2k-1)L + 2jL\} \\ &= \{L + 2L(j-k)\}, \end{aligned} \quad (6.90)$$

i.e.

$$S_k(t) \stackrel{(6.88)}{=} S_k(\tau_e) \stackrel{(6.89),(6.90)}{=} Q(\tau_e) + 2L(j-k) \stackrel{(6.88)}{=} Q(t) + 2L(j-k).$$

If $j \in 2\mathbb{Z} + k + 1 \setminus \{0\}$ by Assertion 6.4 and (6.78) it follows that

$$\begin{aligned} S_k(t) &= S_k(\tau_e) \in [-(2k-1)L + 2(j-1)L, -(2k-1)L + 2jL] \cap \bigcup_{i \in \mathbb{Z}} \{(4i+1)L\} \cap I_k \\ &= \{-(2k-1)L + 2(j-1)L\} \\ &= \{-L + 2L(j-k)\}, \end{aligned} \quad (6.91)$$

which gives

$$S_k(t) \stackrel{(6.88)}{=} S_k(\tau_e) \stackrel{(6.91),(6.89)}{=} -Q(\tau_e) + 2L(j-k) \stackrel{(6.88)}{=} -Q(t) + 2L(j-k).$$

We proceed similar if $j = 0$ or $Q(\tau_e) = -L$, and all in all Lemma 6.1 follows. \square

As mentioned before, we may determine the distribution of $S_{k,t}$ for $t \rightarrow \infty$, if we find a stationary Markov process which contains $S_k(t)$ - or by Lemma 6.1: which contains $Q(t)$ and $j_k(t)$. But since the value of $j_k(0)$ is determined, to obtain a Markov process with stationary measure we have to introduce a more general process such that “ $j_k(0)$ ” may take any $j \in \mathcal{J}_k$ (cf. (6.14)).

Denote by

$$j_k^l(t) \in \mathcal{J}_k$$

the random variable which is the number of the subinterval (cf. (6.12)) in which

$$S_k^l(t) := \left((-1)^{2k+l} S_k(t) + 2Ll \right) \bmod I_k, \quad l \in \{-k, -k+1, \dots, k-1\} \quad (6.92)$$

is at time t . Note that $j_k^l(0) = k + l$ by definition of $S_k^l(t)$ and for $l = 0$, $S_k^l(t) = S_k(t)$ (cf. (6.8)), i.e. $j_k^0(t) = j_k(t)$ with $j_k(t)$ defined in (6.14).

Further we introduce the process $\tilde{S}_k(t)$, where $\tilde{j}_k(t) \in \mathcal{J}_k$ is the number of the subinterval (cf. (6.12)) where $\tilde{S}_k(t)$ is at time t . $\tilde{S}_k(t)$ is defined as (6.92) but the value of $\tilde{j}_k(0)$ is distributed according to some initial distribution (counting measure) $\tilde{\rho}_l$.

We now prove that $\tilde{S}_k(t)$ is a function of $Q(t)$ and $\tilde{j}_k(t)$.

Corollary 6.1. For any $t \geq 0$, $\tilde{S}_k(t)$ is determined by $Q(t)$ and $\tilde{j}_k(t)$ by the function

$$\begin{aligned} f : [-L, L] \times \mathcal{J}_k &\rightarrow I_k, \\ (Q(t), \tilde{j}_k(t)) &\mapsto \tilde{S}_k(t) \end{aligned} \quad (6.93)$$

where f is given in Lemma 6.1.

Proof of Corollary 6.1. We show that $S_k^l(t)$ as defined in (6.92) is determined by $j_k^l(t)$ and $Q(t)$ by the function f as given in Lemma 6.1, i.e.

$$S_k^l(t) = \begin{cases} Q(t) + 2L(j_k^l(t) - k) & , \text{ if } j_k^l(t) \in (2\mathbb{Z} + k) \setminus \{0\} \\ -Q(t) + 2L(j_k^l(t) - k) & , \text{ if } j_k^l(t) \in (2\mathbb{Z} + k + 1) \setminus \{0\}. \\ Q(t) - 2kL & , \text{ if } j_k^l(t) = 0 \in 2\mathbb{Z} + k, Q(t) \in [0, L] \\ Q(t) + 2kL & , \text{ if } j_k^l(t) = 0 \in 2\mathbb{Z} + k, Q(t) \in [-L, 0) \\ -Q(t) + 2kL & , \text{ if } j_k^l(t) = 0 \in 2\mathbb{Z} + k + 1, Q(t) \in [0, L] \\ -Q(t) - 2kL & , \text{ if } j_k^l(t) = 0 \in 2\mathbb{Z} + k + 1, Q(t) \in [-L, 0). \end{cases} \quad (6.94)$$

By that, Corollary 6.1 follows immediately, since f doesn't differ in l .

We consider in the following that

$$j_k^l(t) \neq 0. \quad (6.95)$$

The proof for the cases where $j_k^l(t) = 0$ follow analogously.

Consider

$$l \in 2\mathbb{Z}. \quad (6.96)$$

Then, we obtain for $S_k^l(t)$ that

$$S_k^l(t) \stackrel{(6.92)}{=} (S_k(t) + 2Ll) \bmod I_k. \quad (6.97)$$

Since $S_k^l(t)$ moves at any time in the same direction as $S_k(t)$ but with a distance of $2lL$,

we have that

$$j_k^l(t) = (j_k(t) + l) \bmod 2k. \quad (6.98)$$

By Lemma 6.1 we obtain for (6.97) that

$$S_k^l(t) \stackrel{(6.92)}{=} (f(Q(t), j_k(t)) + 2Ll) \bmod I_k. \quad (6.99)$$

We now show that

$$j_k^l(t) \in 2\mathbb{Z} + k \Leftrightarrow j_k(t) \in 2\mathbb{Z} + k \quad (6.100)$$

and

$$j_k^l(t) \in 2\mathbb{Z} + k + 1 \Leftrightarrow j_k(t) \in 2\mathbb{Z} + k + 1. \quad (6.101)$$

We start with “ \Rightarrow ” of (6.100). Since (6.96), there is a $n \in \mathbb{Z}$ such that

$$l = 2n \quad (6.102)$$

and we have that for some $p \in \mathbb{Z}$

$$j_k^l(t) \stackrel{(6.98)}{=} (j_k(t) + l) \bmod 2k \stackrel{(6.102)}{=} (j_k(t) + 2n) \bmod 2k = j_k(t) + 2n - p2k. \quad (6.103)$$

If $j_k^l(t) \in 2\mathbb{Z} + k$, i.e. there is a $m \in \mathbb{Z}$ such that

$$j_k^l(t) = 2m + k,$$

we obtain by (6.103) that

$$j_k(t) + 2n - p2k = 2m + k \Leftrightarrow j_k(t) = 2(m - n + p) + k. \quad (6.104)$$

Since $m - n + p \in \mathbb{Z}$ the r.h.s. of (6.100) follows.

Now we show “ \Leftarrow ” of (6.100). Consider $j_k(t) \in 2\mathbb{Z} + k$, i.e. there is a $m \in \mathbb{Z}$ such that

$$j_k(t) = 2m + k. \quad (6.105)$$

We use again (6.103) and we obtain that

$$\begin{aligned} j_k^l(t) &\stackrel{(6.103)}{=} j_k(t) + 2n - p2k \\ &\stackrel{(6.105)}{=} 2m + k + 2n - p2k \\ &= 2(m + n - pk) + k, \end{aligned} \quad (6.106)$$

which gives that

$$j_k^l(t) \in 2\mathbb{Z} + k.$$

(6.104) and (6.106) give (6.100). (6.101) follows by the same arguments. All in all we obtain for (6.99) by (6.100) and (6.101) that with (6.96)

$$S_k^l(t) = \begin{cases} (Q(t) + 2L(j_k(t) - k) + 2lL) \bmod I_k & , \text{ if } j_k(t) \in 2\mathbb{Z} + k \\ (-Q(t) + 2L(j_k(t) - k) + 2lL) \bmod I_k & , \text{ if } j_k(t) \in 2\mathbb{Z} + k + 1. \end{cases}$$

$$\stackrel{(6.98)}{=} \begin{cases} Q(t) + 2L(j_k^l(t) - k) & , \text{ if } j_k^l(t) \in 2\mathbb{Z} + k \\ -Q(t) + 2L(j_k^l(t) + l - k) & , \text{ if } j_k^l(t) \in 2\mathbb{Z} + k + 1. \end{cases}$$

Now let

$$l \in 2\mathbb{Z} + 1, \tag{6.107}$$

i.e. there is a $n \in \mathbb{Z}$ such that

$$l = 2n + 1. \tag{6.108}$$

With (6.108) we have that

$$S_k^l(t) \stackrel{(6.92)}{=} (-S_k(t) + 2Ll) \bmod I_k, \tag{6.109}$$

i.e. since $S_k^l(t)$ moves in opposite direction as $S_k(t)$ and $S_k^l(t)$ starts in $j_k^l(0) = k + l$ with distance $2lL$ to $S_k(0)$, we have that

$$j_k^l(t) = (k + l - (j_k(t) - k)) \bmod 2k = (2k - j_k(t) + l) \bmod 2k. \tag{6.110}$$

By Lemma 6.1 we have for (6.109) that

$$S_k^l(t) \stackrel{(6.92)}{=} - (f(Q(t), j_k(t)) + 2Ll) \bmod I_k$$

$$= \begin{cases} -(Q(t) + 2L(j_k(t) - k) + 2lL) \bmod I_k & , \text{ if } j_k(t) \in 2\mathbb{Z} + k \\ -(-Q(t) + 2L(j_k(t) - k) + 2lL) \bmod I_k & , \text{ if } j_k(t) \in 2\mathbb{Z} + k + 1 \end{cases}$$

$$= \begin{cases} (-Q(t) + 2L(-j_k(t) + k - l)) \bmod I_k & , \text{ if } j_k(t) \in 2\mathbb{Z} + k \\ (Q(t) + 2L(-j_k(t) + k - l)) \bmod I_k & , \text{ if } j_k(t) \in 2\mathbb{Z} + k + 1. \end{cases} \tag{6.111}$$

Now we show that

$$j_k^l(t) \in 2\mathbb{Z} + k \Leftrightarrow j_k(t) \in 2\mathbb{Z} + k + 1 \tag{6.112}$$

and

$$j_k^l(t) \in 2\mathbb{Z} + k + 1 \Leftrightarrow j_k(t) \in 2\mathbb{Z} + k. \quad (6.113)$$

We show “ \Rightarrow ” of (6.112). We have that

$$\begin{aligned} j_k^l(t) &\stackrel{(6.110)}{=} (2k - j_k(t) + l) \bmod 2k \\ &\stackrel{(6.108)}{=} (2k - j_k(t) + 2n + 1) \bmod 2k \\ &= 2k - j_k(t) + 2n + 1 - p2k, \end{aligned} \quad (6.114)$$

for some appropriate $p \in \mathbb{Z}$. Consider $j_k^l(t) \in 2\mathbb{Z} + k$, i.e. there is a $m \in \mathbb{Z}$ such that

$$j_k^l(t) = 2m + k. \quad (6.115)$$

By (6.114) and (6.115) $j_k(t)$ has to be such that

$$\begin{aligned} 2k - j_k(t) + 2n + 1 - p2k &= 2m + k \\ \Leftrightarrow j_k(t) &= k + 2n - 2m + 1. \end{aligned}$$

i.e.

$$j_k(t) \in 2\mathbb{Z} + k + 1.$$

We show “ \Leftarrow ” of (6.112). Consider

$$j_k(t) \in 2\mathbb{Z} + k + 1,$$

i.e. there is a $m \in \mathbb{Z}$ such that

$$j_k(t) \in 2m + k + 1. \quad (6.116)$$

Plugging (6.116) into (6.114) gives

$$\begin{aligned} j_k^l(t) &\stackrel{(6.114)}{=} 2k - j_k(t) + 2n + 1 - p2k \\ &\stackrel{(6.116)}{=} 2k - 2m + k + 1 + 2n + 1 - p2k \\ &= 2(k - m + 1 + n - pk) + k, \end{aligned}$$

which gives

$$j_k^l(t) \in 2\mathbb{Z} + k.$$

This ends the proof of (6.112). (6.113) follows by the same arguments.

By (6.112) and (6.113) we finally obtain for (6.111) with (6.107) that

$$S_k^l(t) = \begin{cases} (-Q(t) + 2L(-j_k(t) + k - l)) \bmod I_k & , \text{ if } j_k(t) \in 2\mathbb{Z} + k \\ (Q(t) + 2L(-j_k(t) + k - l)) \bmod I_k & , \text{ if } j_k(t) \in 2\mathbb{Z} + k + 1. \end{cases}$$

$$\stackrel{(6.110)}{=} \begin{cases} Q(t) + 2L(j_k^l(t) - k) & , \text{ if } j_k^l(t) \in 2\mathbb{Z} + k \\ -Q(t) + 2L(j_k^l(t) - k) & , \text{ if } j_k^l(t) \in 2\mathbb{Z} + k + 1. \end{cases}$$

This gives (6.94) for the case (6.95). Recall that the remaining cases can be proven by similar arguments.

We have shown in (6.94) that for any $l \in \{-k, -k + 1, \dots, k - 1\}$

$$S_k^l(t) = f(Q(t), j_k^l(t))$$

where f is given in Lemma 6.1. □

We now define the process $\tilde{\mathcal{M}}_{k,t}$ which contains $Q(t)$ and $\tilde{j}_k(t)$ and by which we determine the distribution of $S_{k,t}$ (cf. (6.7)) for $t \rightarrow \infty$.

We consider the process

$$\tilde{\mathcal{M}}_{k,t} := \{Z_k(t)\}_{t \in \mathbb{R}^+} \tag{6.117}$$

with

$$Z_k(t) := \left(Q(t), V(t), q_i(t), v_i(t), \tilde{j}_k(t) \right), \tag{6.118}$$

where $\tilde{j}_k(t)$ is defined underneath (6.92). The process is defined on $\hat{\Omega} \times \mathcal{J}_k$ (cf. (2.3), (6.14)) with state space $\hat{\Omega}|_{\Lambda} \times \mathcal{J}_k$, where $\hat{\Omega}|_{\Lambda}$ is the set of all configurations of the particles in Λ .

Lemma 6.2. The process $\tilde{\mathcal{M}}_{k,t}$ as defined in (6.117) is a Markov process with stationary measure

$$\Pi_k(dz) = \mu \times \rho_{j_k}(Z_k(0) \in dz), \tag{6.119}$$

where μ is given in (2.9) and ρ_{j_k} is the counting measure with equal weight for any $j \in \mathcal{J}_k$ (cf. (6.14)).

Proof of Lemma 6.2. The Markov property of $\tilde{\mathcal{M}}_{k,t}$ follows by the same reasoning which we used to prove Lemma 5.1. Note that the evolution of $\tilde{j}_k(t)$ is apart from the incoming

atoms deterministic. Further, $\{\tilde{j}_k(t), t > \tau\}$ is determined by

$$Z_k(\tau) = (Q(\tau), V(\tau), q_i(\tau), v_i(\tau), \tilde{j}_k(\tau))$$

and all atoms entering Λ after time τ : $\{\tilde{j}_k(t), t > \tau\}$ is determined by $\{\tilde{S}_k(t), t > \tau\}$. $\{\tilde{S}_k(t), t > \tau\}$ is determined by $\tilde{S}_k(\tau)$ and the incoming atoms after time τ . Since $\tilde{S}_k(\tau)$ is a function of $Z_k(\tau)$ (cf. Corollary 6.1), $\{\tilde{j}_k(t), t > \tau\}$ is determined by $Z_k(\tau)$ and all atoms entering after time τ .

To show the stationarity we make use of the *Skew-Product-Lemma* 4.2. We consider \mathcal{X} to be the phase space of the system of all particles, i.e.

$$\mathcal{X} = \hat{\Omega}$$

(cf. (2.3)). The measure ξ is the product of ideal gas measure with Gibbs measure of the molecule, i.e.

$$\xi = \mu$$

given in (2.9). Let

$$\mathcal{Y} = \mathcal{J}_k$$

with \mathcal{J}_k given in (6.14).

We consider the evolution

$$\tilde{\Psi}_t(\hat{\omega}, j) := \left(\Phi_t(\hat{\omega}), \chi_t^{(\hat{\omega})}(j) \right), \quad \hat{\omega} \in \hat{\Omega}, j \in \mathcal{J}_k, \quad (6.120)$$

where Φ_t is the dynamical evolution of the system of all particles (cf. (2.10)), and

$$\begin{aligned} \chi_t^{(\hat{\omega})} : \mathcal{J}_k &\rightarrow \mathcal{J}_k, \\ \tilde{j}_k(0) &\mapsto \tilde{j}_k(t). \end{aligned}$$

To prove the stationarity of $\tilde{\mathcal{M}}_{k,t}$ w.r.t. the measure given in (6.119), by the *Skew-Product-Lemma* it is enough to show that $\chi_t^{(\hat{\omega})}$ preserves ρ_{j_k} , what we show now. Define $A_{j,i} \subset \hat{\Omega}$ with

$$A_{j,i} := \left\{ \hat{\omega} : \tilde{j}_k(0) = j \Rightarrow \tilde{j}_k(t) = \begin{cases} j+i & , \text{ if } i \leq 2k-1-j \\ j+i-2k & , \text{ if } i > 2k-1-j \end{cases} \right\}$$

with $i \in \{0, 1, \dots, 2k-1\}$. The set $A_{j,i}$ includes all the initial conditions for which the value of \tilde{j}_k “grows” (in mod $2k$) by i steps during $[0, t]$ if $\tilde{j}_k(0) = j$. Since *the value of \tilde{j}_k has no affect on the evolution of the particles*, it follows by the dynamics of $\tilde{j}_k(t)$ that

$$A_{j,i} = A_{j',i} \quad (6.121)$$

if $j' \in j + 2\mathbb{Z}$ and

$$A_{j,i} = A_{j',-i} \quad (6.122)$$

if $j' \in j + (2\mathbb{Z} + 1)$. Note that for given $j \in \mathcal{J}_k$

$$A_{j,i} \cap A_{j,i'} = \emptyset \text{ for } i \neq i', \text{ and } \bigcup_{i=0}^{2k-1} A_{j,i} = \hat{\Omega}.$$

Consider now $\hat{\omega} \in A_{j,i}$ for some given $i \in \{0, \dots, 2k-1\}, j \in \mathcal{J}_k$, then with (6.121) and (6.122) either

$$\left(\chi_t^{(\hat{\omega})}\right)^{-1}(j'') = \begin{cases} j'' - i & , \text{ if } j'' \geq i \\ j'' - i + 2k & , \text{ if } j'' < i \end{cases} \quad (6.123)$$

or

$$\left(\chi_t^{(\hat{\omega})}\right)^{-1}(j'') = \begin{cases} j'' + i & , \text{ if } j'' \leq 2k - 1 - i \\ j'' + i - 2k & , \text{ if } j'' > 2k - 1 - i \end{cases} \quad (6.124)$$

i.e. if (6.123) and $j'' \geq i$ we obtain that

$$\rho_{j_k} \left(\left(\chi_t^{(\hat{\omega})}\right)^{-1}(j'') \right) \stackrel{(6.123)}{=} \rho_{j_k}(j'' - i) = \rho_k(j'') \quad (6.125)$$

and if $j'' < i$ that

$$\rho_{j_k} \left(\left(\chi_t^{(\hat{\omega})}\right)^{-1}(j'') \right) \stackrel{(6.123)}{=} \rho_{j_k}(j'' - i + 2k) = \rho_k(j''). \quad (6.126)$$

Note that the last equation in (6.125) resp. in (6.126) follows since ρ_{j_k} is the counting measure with equal weight to any $j \in \mathcal{J}_k$. By the same arguments we obtain that if (6.124) and $j'' \leq 2k - 1 - i$ that

$$\rho_{j_k} \left(\left(\chi_t^{(\hat{\omega})}\right)^{-1}(j'') \right) = \rho_k(j'') \quad (6.127)$$

and if $j'' > 2k - 1 - i$ that

$$\rho_{j_k} \left(\left(\chi_t^{(\hat{\omega})}\right)^{-1}(j'') \right) = \rho_k(j''). \quad (6.128)$$

Since (6.123), (6.124), (6.125), (6.126), (6.127) and (6.128) hold for any $j \in \mathcal{J}_k$ and any $i \in \{0, 1, \dots, 2k-1\}$ it follows that $\chi_t^{(\hat{\omega})}$ preserves ρ_{j_k} . Finally, we consider

$$\theta = \rho_{j_k},$$

and we obtain by the *Skew-Product-Lemma* that $\tilde{\Psi}_t$ (cf. (6.120)) preserves the measure

$$\mu \times \rho_{j_k}.$$

Now consider the extended probability space

$$\Sigma_{j_k} := \left(\hat{\Omega} \times \mathcal{J}_k, \mathcal{F} \times \mathcal{P}(\mathcal{J}_k), \mu \times \rho_{j_k} \right).$$

Since $Z_k(t)$ (cf. (6.118)) is a function of $\tilde{\Psi}_t$ (cf. (6.120)), which is a measure preserving transformation on Σ_{j_k} , the stationary measure of $\tilde{\mathcal{M}}_{k,t}$ (cf. (6.117)) is

$$\Pi_k(dz) = \mu \times \rho_{j_k}(Z_k(0) \in dz).$$

With that Lemma 6.2 follows. □

To determine the distribution of $S_{k,t}$ for $t \rightarrow \infty$ we use following Lemma. Denote by $\Pi_{k,z}^t$, $z \in \hat{\Omega}|_{\Lambda} \times \mathcal{J}_k$ the transition probability of the process $\tilde{\mathcal{M}}_{k,t}$ (cf. (6.117)). Let ϕ be an initial distribution, then $\phi \Pi_k^t(\cdot) = \int \phi(dz) \Pi_{k,z}^t(\cdot)$ is the distribution at time t of $\tilde{\mathcal{M}}_{k,t}$ starting in ϕ .

Lemma 6.3. Consider the process $\tilde{\mathcal{M}}_{k,t}$ as defined in (6.117). Then,

$$\|\phi \Pi_k^t - \mu \times \rho_{j_k}\| \rightarrow 0 \text{ as } t \rightarrow \infty,$$

where ϕ is an initial distribution and $\mu \times \rho_{j_k}$ is given in (6.119).

Note, since $S_k(t)$ is a function of $Q(t)$ and $\tilde{j}_k(t)$ (given $\tilde{j}_k(0) = k$) (cf. Assertion 6.1) and since $\tilde{\mathcal{M}}_{k,t}$ contains these variables, by Lemma 6.3 we then obtain the distribution of $S_{k,t}$ for $t \rightarrow \infty$ by choosing the appropriate initial measure ϕ . Before we show this, we prove Lemma 6.3.

The idea of proving Lemma 6.3 is the following: We make use of the *Harris Theorem* (see [GLR82]):

Let (Γ, π, P) be an ergodic, aperiodic Harris chain with stationary distribution π . Then, for $n \in \mathbb{N}$ and π a.e. $\xi \in \Gamma$

$$\|P_\xi^n - \pi\| \rightarrow 0, \text{ as } n \rightarrow \infty. \tag{6.129}$$

For the definition of ergodicity, aperiodicity and Harris see [GLR82]. To make use of the *Harris Theorem* we consider $\tilde{\mathcal{M}}_{k,t}$ in discrete time: Let $\tau > 0$. Then, $\tilde{\mathcal{M}}_{k,t}$ is observed only at times which are integer multiples of τ , which defines the Markov process $\tilde{\mathcal{M}}_{k,n\tau} = \{Z_k(n\tau)\}_{n \in \mathbb{N}}$ for any $\tau > 0$ with transition probability $\Pi_{k,z}^t, t \in \tau\mathbb{N}$ and stationary measure $\mu \times \rho_{j_k}$ (cf. (6.119)). Proving that $\tilde{\mathcal{M}}_{k,n\tau}$ is an ergodic, aperiodic Harris chain for any $\tau > 0$, we follow essentially the arguments in [GLR82], who showed Harris mixing, i.e. (6.129), of a related Markov process.

To show that $\tilde{\mathcal{M}}_{k,n\tau}$ is an ergodic, aperiodic Harris chain for any $\tau > 0$, it is enough to establish following lemma, which is about the continuous Markov process $\tilde{\mathcal{M}}_{k,t}$ (cf. (6.117)).

Let $\tilde{\mathbb{P}}_k$ denote the path measure induced by $\tilde{\mathcal{M}}_{k,t}$ and let $\tilde{\mathbb{P}}_{k,z}$ denote the conditional path measure given $Z_k(0) = z, z \in \hat{\Omega}|_{\Lambda} \times \mathcal{J}_k$.

Lemma 6.4. There exists a set $\bar{\Omega} \subset \hat{\Omega}|_{\Lambda} \times \mathcal{J}_k$ with $\mu \times \rho_{j_k}(\bar{\Omega}) = 1$, such that the family of measures $\{\mathbb{P}_{k,z}(\mathrm{d}\tilde{V}_2, \mathrm{d}\tilde{\tau}_2), \mathbb{P}_{k,z'}(\mathrm{d}\tilde{V}_2, \mathrm{d}\tilde{\tau}_2); z, z' \in \bar{\Omega}\}$ are overlapping, where $\tilde{\tau}_2$ is a time where the molecule is alone and $Q(\tilde{\tau}_2) = L$ and $\tilde{j}_k(\tilde{\tau}_2) = k, V(\tilde{\tau}_2) = \tilde{V}_2$.

See [GLR82] for the definition of overlap of a family of measures.

Since the strategy of the proof is the same as in Section 5.2, we shall only point out some essential changes which arise from observing the process on the torus $I_k, k \in \mathbb{N}$ (which is arbitrary large with growing k), followed by some ideas how to establish overlap.

Proof of Lemma 6.4. Let $\bar{\Omega} = \{z \in \hat{\Omega}|_{\Lambda} \times \mathcal{J}_k : \tau_1 < \infty \text{ } \mathbb{P}_z \text{ a.s.}\}$, where τ_1 is the time, when for the first time the molecule hits the wall at L and is alone in the interval. From Theorem A in Appendix A in [GLR82], it follows that

$$\mu \times \rho_{j_k}(\bar{\Omega}) = 1. \tag{6.130}$$

Note since in our model the atoms lie to both sides of the molecule, we have to modify set A in the proof of Theorem A in [GLR82] slightly as follows. First, we send in one sufficiently large atom from the right, such that the molecule pushes all atoms to its left out of the interval. Then, we are in the same situation as in [GLR82], and continue as in [GLR82], to show (6.130).

The arguments that the family of measures

$$\{\mathbb{P}_{k,z}(\mathrm{d}\tilde{V}_2, \mathrm{d}\tilde{\tau}_2), \mathbb{P}_{k,z'}(\mathrm{d}\tilde{V}_2, \mathrm{d}\tilde{\tau}_2), z, z' \in \bar{\Omega}\}$$

are overlapping, are similar as in the proof of Overlap-Lemma 5.2: Besides the particles in the interval, one now has to control the value of $\tilde{j}_k(t)$ instead of the value of $\sigma(t)$. On the one hand the argumentation is even simpler, since only pairwise overlapping is required (we don't need an explicit overlap set, which in Overlap-Lemma 5.2 is necessary to give an explicit rate). The requirement of pairwise overlapping allows to choose \mathcal{V}_2 , the set of molecular velocity at time τ_2 , dependent on $\tau_1, V_1, \tau'_1, V'_1$, which makes it easier to find an overlap set for $\mathbb{P}_{k,z}(\mathrm{d}\tilde{V}_2\mathrm{d}\tilde{\tau}_2)$ and $\mathbb{P}_{k,z'}(\mathrm{d}\tilde{V}_2\mathrm{d}\tilde{\tau}_2)$. On the other hand there is one more difficulty, since we have to control the value of \tilde{j}_k , which is the number of the subinterval where \tilde{S}_k "is" at a certain time. The larger k , the larger the torus I_k (cf. (6.6)), i.e. the more possibilities for the position of \tilde{S}_k , i.e. the larger k , the later the overlap may occur. But since \tilde{S}_k , i.e. \tilde{j}_k is periodic on the torus I_k , one can show that overlap occurs in finite time.

We give some ideas how to construct an overlap set. Consider $Z_k(0) = z \in \bar{\Omega}$. Denote by $\tilde{\tau}_1$ the time, when the molecule is alone in Λ , $Q(\tilde{\tau}_1) = L$ and $\tilde{j}_k(\tilde{\tau}_1) \in \{k, k+1\}$ (i.e. by Corollary 6.1 $\tilde{S}_k(t) = L$) for the first time after $t = 0$ and recall that τ_1 is the time when the molecule is alone with $Q(\tau_1) = L$ (no requirement on $\tilde{j}_k(\tau_1)$). Then, either

$$\tau_1 = \tilde{\tau}_1$$

or

$$\tilde{\tau}_1 > \tau_1.$$

In the latter case, i.e. if $\tilde{j}_k(\tau_1) \notin \{k, k+1\}$, we consider the event that no atom enters Λ between τ_1 and $\tilde{\tau}_1$. Let $V_1 := V(\tau_1)$. Then, since $\tilde{S}_k(t)$ is periodic on I_k , latest at time

$$\tau_1 + \frac{(2k-1)4L}{|V_1|}$$

$\tilde{S}_k(t)$ is in $[-L, L]$, i.e.

$$\tilde{\tau}_1 < \tau_1 + \frac{(2k-1)4L}{|V_1|} < \infty.$$

the latter follows since $|V_1| > 0$. Denote by $\tilde{V}_1, \tilde{\sigma}_1$ the value of V resp. σ at time $\tilde{\tau}_1$. Now we distinguish two scenarios.

Scenario I: If $\tilde{j}_k(\tilde{\tau}_1) = k+1$ (i.e. \tilde{S}_k "goes through L from left to right"), we send in an atom from the left such that the molecular post collision velocity $V' > 0$. The collision shall take place after the molecule was at L , but before the molecule reaches $-L$ the first time after $\tilde{\tau}_1$. Let $\tilde{\tau}_2$ be the time, when the molecule reaches L again.

Scenario II: If $\tilde{j}_k(\tilde{\tau}_1) = k$ (i.e. \tilde{S}_k "goes through L from right to left"), we send in a very fast atom from the left, such that $V' > \delta > 0$ where δ is some positive constant, and before the molecule reaches $-L$ the first time after $\tilde{\tau}_1$. Then, we send in a second atom from the

left, such that the collision takes place after the molecule is reflected at L and before it reaches $-L$, and such that $V' > 0$. Let $\tilde{\tau}_2$ be the time, when the molecule reaches L the first time after the second collision.

Note that in Scenario I one has to pay attention to virtual collisions. Let v be the velocity of the incoming atom. If $|v| < |\tilde{V}_1|$, the interval of collision time described above (collision takes place after the molecule was at L , but before it reaches $-L$) has to be limited, otherwise the atom has to be in Λ before $\tilde{\tau}_1$ to reach the molecule in time, which is not possible. Since in Scenario II the necessary atoms are both very fast (one chooses δ large enough), virtual collisions doesn't play any role here.

Choosing δ large enough, by elementary calculations one obtains that one can send in the atoms in both scenarios such that for equal $\tilde{V}_1, \tilde{\tau}_1$ the molecule is alone in Λ and reaches L at equal time

$$\tilde{\tau}_2 \in \left(\max \left\{ \tilde{\tau}_1 + \frac{L}{|\tilde{V}_1|} + \frac{L}{|\tilde{V}_2|}, \tilde{\tau}_1 + \frac{2L}{|\tilde{V}_2|} \frac{2m}{M+m} \right\}, \tilde{\tau}_1 + \frac{2L}{|\tilde{V}_1|} + \frac{2L}{|\tilde{V}_2|} \right), \quad (6.131)$$

with equal \tilde{V}_2 where \tilde{V}_2 may take any value with

$$\tilde{V}_2 < 0. \quad (6.132)$$

To establish pairwise overlap, the $(\tilde{V}_2, \tilde{\tau}_2)$ -sets defined by (6.131) and (6.132) with $|\tilde{V}_1| > 0, \tilde{\tau}_1 < \infty$, have to be pairwise non-disjoint for any $\tilde{V}_1, \tilde{V}_1' < 0$ and any finite $\tilde{\tau}_1, \tilde{\tau}_1'$. This is the case if there is a \tilde{V}_2 -set

$$\mathcal{V}_2 := (a, b) \subset (-\infty, 0) \quad (6.133)$$

such that

$$\max \left\{ \tilde{\tau}_1 + \frac{L}{|\tilde{V}_1|} + \frac{L}{|\tilde{V}_2|}, \tilde{\tau}_1 + \frac{2L}{|\tilde{V}_2|} \frac{2m}{M+m} \right\} < \tilde{\tau}_1' + \frac{2L}{|\tilde{V}_1'|} + \frac{2L}{|\tilde{V}_2|}$$

and

$$\max \left\{ \tilde{\tau}_1' + \frac{L}{|\tilde{V}_1'|} + \frac{L}{|\tilde{V}_2|}, \tilde{\tau}_1' + \frac{2L}{|\tilde{V}_2|} \frac{2m}{M+m} \right\} < \tilde{\tau}_1 + \frac{2L}{|\tilde{V}_1|} + \frac{2L}{|\tilde{V}_2|}$$

for any $\tilde{V}_2 \in \mathcal{V}_2$. This is true for $|\tilde{V}_2|$ small enough, and since a, b in (6.133) can be chosen arbitrary close to zero, Lemma 6.4 follows by an appropriate choice of \mathcal{V}_2 . \square

From the overlap in the path measures we obtain overlap for the transition probabilities. Referring to [GLR82] we formulate

Lemma 6.5. (i) For any $z_1, z_2 \in \bar{\Omega} \Pi_{k,z_1}^t, \Pi_{k,z_2}^t$ are overlapping for t sufficiently large.

(ii) For any $z \in \bar{\Omega} \Pi_{k,z}^t$ and Π_k are overlapping for t sufficiently large.

For the proof of Lemma 6.5 we can refer to the proof given in [GLR82] or to the arguments we used in the proof of Lemma 5.8.

By the same reference we have the following lemma, which follows from Lemma 6.5 (see [GLR82]).

Lemma 6.6. For any $\tau > 0$ the process $\tilde{\mathcal{M}}_{k,n\tau}$ as defined underneath (6.129) is an aperiodic, ergodic Harris chain.

Finally, by Lemma 6.6 we can prove Lemma 6.3.

Proof of Lemma 6.3. By Lemma 6.6 and the *Harris Theorem* we obtain for $n \in \mathbb{N}$ that

$$\|\Pi_{k,z}^{n\tau} - \mu \times \rho_{j_k}\| \rightarrow 0 \text{ as } n \rightarrow \infty$$

for $\mu \times \rho_{j_k}$ a. e. $z \in \hat{\Omega}|_{\Lambda} \times \mathcal{J}_k$. By Corollary 1 in [GLR82] it follows for $t \in \mathbb{R}^+$ that

$$\|\phi \Pi_k^t - \mu \times \rho_{j_k}\| \rightarrow 0 \text{ as } t \rightarrow \infty,$$

where ϕ is a initial distribution of the process. □

Now we can determine the distribution of $S_{k,t}$ (cf. (6.7)) for $t \rightarrow \infty$, using Lemma 6.3. Denote by $\mathcal{P}_{k,t}$ the image measure of $S_k(t)$. Then, since $S_k(t)$ is a function of $Q(t), \tilde{j}_k(t)$ with $\tilde{j}_k(0) = k$ (cf. Lemma 6.1) choosing

$$\phi_{S_k} := \mu \times \rho_{\{k\}},$$

where $\rho_{\{k\}}$ is the counting measure such that $\tilde{j}_k(0) = k$ with probability 1, we have that

$$\mathcal{P}_{k,t}((a, b)) = \phi_{S_k} \Pi_k^t(f(Q(t), \tilde{j}_k(t)) \in (a, b)) \tag{6.134}$$

with f given in (6.93). By Lemma 6.3 it follows with (6.134) that

$$\lim_{t \rightarrow \infty} \mathcal{P}_{k,t}((a, b)) = \mu \times \rho_{j_k}(f(Q, j) \in (a, b)). \tag{6.135}$$

We now show that with (6.135) $S_{k,t}$ is distributed uniformly on I_k for $t \rightarrow \infty$ for any $k \in \mathbb{N}$.

Assertion 6.7. Let $k \in \mathbb{N}$. Consider f as defined in (6.93), I_k as given in (6.6) and $\mu \times \rho_{j_k}$ given in (6.119). Let $E \in \mathbb{R}$, then

$$\mu \times \rho_{j_k}(f(Q, j) \leq E) = \begin{cases} \frac{E+2kL}{4kL} & , \text{ if } -2kL \leq E \leq 2kL \\ 0 & , \text{ if } E < -2kL \\ 1 & , \text{ if } E > 2kL. \end{cases} \quad (6.136)$$

Proof of Assertion 6.7. Consider $-2kL \leq E \leq 2kL$. To determine $\mu \times \rho_{j_k}(f(Q, j) \leq E)$, we first determine

$$A_{\leq E} := \{(Q, j) : f(Q, j) \leq E\}. \quad (6.137)$$

Note that the case where $j = 0$ is a special case, since this subinterval with number 0 is splitted (cf. (6.13)). Therefore, we distinguish the following cases.

If $-2kL \leq E \leq -2kL + L$, then

$$A_{\leq E} = \{Q \in [0, E+2kL] \wedge j = 0, \text{ if } k \in 2\mathbb{Z}; Q \in [-(E+2kL), 0] \wedge j = 0, \text{ if } k \in 2\mathbb{Z}+1\}$$

and

$$\mu \times \rho_{j_k}(A_{\leq E}) = \frac{E+2kL}{2L} \frac{1}{2k} = \frac{E+2kL}{4kL}. \quad (6.138)$$

If $-2kL + L < E \leq 2kL$, then

$$\{(Q, j) : Q \in [0, L] \wedge j = 0, \text{ if } k \in 2\mathbb{Z}; Q \in [-L, 0] \wedge j = 0, \text{ if } k \in 2\mathbb{Z}+1\} \subset A_{\leq E} \quad (6.139)$$

To determine the remaining (Q, j) -subsets of $A_{\leq E}$, note that for given $j \in \mathcal{J}_k$ with $Q \in [-L, L]$

$$f(Q, j) \leq L + 2L(j - k).$$

Denote by \bar{j} the largest $j \in \{0, \dots, 2k - 1\}$ such that

$$L + 2L(j - k) \leq E. \quad (6.140)$$

That means that for the \bar{j} -th subinterval any value $Q \in [-L, L]$ fulfills that $f(Q, \bar{j}) \leq E$. This is also the case for the j -th subinterval where $0 < j \leq \bar{j}$, but not for $j = 0$ or $j > \bar{j}$.

From (6.140) it follows that

$$\bar{j} = \left\lfloor \frac{E-L}{2L} \right\rfloor + k. \quad (6.141)$$

Then, for any $Q(t) \in [-L, L]$ and $0 < j \leq \bar{j}$

$$f(Q, j) \leq L + 2L(\bar{j} - k) \leq E,$$

i.e.

$$\{(Q, j) : Q \in [-L, L] \wedge 0 < j \leq \bar{j}\} \subset A_{\leq E}. \quad (6.142)$$

Since for $\bar{j} + 1$ not any $Q \in [-L, L]$ is such that $f(Q, \bar{j} + 1) \leq E$ is fulfilled, we determine the values of Q now. Note that if $\bar{j} + 1 = 2k$, then

$$\bar{j} + 1 \equiv 0.$$

Assume that

$$\bar{j} + 1 < 2k.$$

Consider $\bar{j} + 1 \in 2\mathbb{Z} + k$. Then, we have that

$$\begin{aligned} f(Q, \bar{j} + 1) &\stackrel{(6.93)}{=} Q(t) + 2L(\bar{j} + 1 - k) \\ &\stackrel{(6.141)}{=} Q(t) + 2L \left(\left\lfloor \frac{E-L}{2L} \right\rfloor + 1 \right) \end{aligned} \quad (6.143)$$

and

$$\begin{aligned} f(Q, \bar{j} + 1) \leq E &\stackrel{(6.143)}{\Leftrightarrow} Q(t) + 2L \left(\left\lfloor \frac{E-L}{2L} \right\rfloor + 1 \right) \leq E \\ &\Leftrightarrow Q(t) \leq E - 2L \left(\left\lfloor \frac{E-L}{2L} \right\rfloor + 1 \right), \end{aligned}$$

i.e.

$$\left\{ (Q, j) : Q \in \left[-L, E - 2L \left(\left\lfloor \frac{E-L}{2L} \right\rfloor + 1 \right) \right] \wedge j = \bar{j} + 1 \right\} \subset A_{\leq E}. \quad (6.144)$$

Hence, if $\bar{j} + 1 \in 2\mathbb{Z} + k$, $\bar{j} + 1 < 2k$ we obtain for the set $A_{\leq E}$ (cf. (6.137)) by (6.139), (6.142) and (6.144) that

$$\begin{aligned} A_{\leq E} = &\{(Q, j); Q \in [0, L] \wedge j = 0, \text{ if } k \in 2\mathbb{Z}; Q \in [-L, 0] \wedge j = 0, \text{ if } k \in 2\mathbb{Z} + 1\} \cup \\ &\cup \{(Q, j) : Q \in [-L, L]\} \wedge 0 < j \leq \bar{j}\} \cup \end{aligned}$$

$$\cup \left\{ (Q, j) : Q \in \left[-L, E - 2L \left(\left\lfloor \frac{E-L}{2L} \right\rfloor + 1 \right) \right] \wedge \bar{j} + 1 \right\} \quad (6.145)$$

With (6.145) we have that

$$\begin{aligned} \mu \times \rho_{j_k}(A_{\leq E}) &= \frac{L}{4kL} + \frac{\bar{j}}{2k} \int_{-L}^L \frac{1}{2L} dQ + \frac{1}{2k} \int_{-L}^{E-2L(\lfloor \frac{E-L}{2L} \rfloor + 1)} \frac{1}{2L} dQ \\ &= \frac{L}{4kL} + \frac{\lfloor \frac{E-L}{2L} \rfloor + k}{2k} + \frac{E - 2L \left(\lfloor \frac{E-L}{2L} \rfloor + 1 \right) + L}{4kL} \\ &= \frac{E + 2kL}{4kL}. \end{aligned} \quad (6.146)$$

We proceed similar if $\bar{j} + 1 \in 2\mathbb{Z} + k + 1$ and obtain that

$$\begin{aligned} A_{\leq E} &= \{(Q, j); Q \in [0, L] \wedge j = 0, \text{ if } k \in 2\mathbb{Z}; Q \in [-L, 0] \wedge j = 0, \text{ if } k \in 2\mathbb{Z} + 1\} \cup \\ &\quad \{(Q, j) : Q \in [-L, L]\} \wedge 0 < j \leq \bar{j}\} \cup \\ &\quad \cup \left\{ (Q, j) : Q \in \left[2L \left(\left\lfloor \frac{E-L}{2L} \right\rfloor + 1 \right) - E, L \right] \wedge \bar{j} + 1 \right\} \end{aligned} \quad (6.147)$$

and

$$\begin{aligned} \mu \times \rho_{j_k}(A_{\leq E}) &\stackrel{(6.147)}{=} \frac{L}{4kL} + \frac{\lfloor \frac{E-L}{2L} \rfloor + k}{2k} + \frac{L - \left(2L \left(\lfloor \frac{E-L}{2L} \rfloor + 1 \right) - E \right)}{4kL} \\ &= \frac{E + 2kL}{4kL}. \end{aligned} \quad (6.148)$$

We obtain by the same methods as used above if $\bar{j} + 1 \in 2\mathbb{Z} + k, \bar{j} + 1 = 2k$ or $\bar{j} + 1 \in 2\mathbb{Z} + k + 1, \bar{j} + 1 = 2k$ that

$$\mu \times \rho_{j_k}(A_{\leq E}) = \frac{E + 2kL}{4kL}.$$

Consider now $E < -2kL$. Then, it follows immediately that

$$A_{\leq E} = \emptyset,$$

i.e.

$$\mu \times \rho_{j_k}(A_{\leq E}) = 0. \quad (6.149)$$

Consider $E > 2kL$. Then, we have that

$$A_{\leq E} = \{(Q, j) : Q \in [-L, L], j \in \{0, \dots, 2k - 1\}\},$$

i.e.

$$\mu \times \rho_{j_k}(A_{\leq E}) = 1. \quad (6.150)$$

Assertion 6.7 follows by (6.138), (6.146), (6.148), (6.149) and (6.150). □

Since $S_k(t)$ (cf. (6.8)) is $S(t)$ (cf. (6.5)) observed on the torus I_k (cf. (6.6)), we can prove, using the distribution of $S_k(t)$ for $t \rightarrow \infty$ given in (6.135), that S_t spreads unboundedly. This is content of the following lemma.

Lemma 6.7. Consider $S(t)$ as defined in (6.5) (with $\sigma(0) = 1$). Then, there exists $\hat{\varepsilon} > 0$ such that for any $E > 0$

$$\sup_t \mu(|S(t)| > E) > \hat{\varepsilon}. \quad (6.151)$$

Proof of Lemma 6.7. Let $E > 0$. Recall that $S(t)$ (cf. (6.5)) and with that $S_k(t)$ (cf. (6.8)) are by definition random variables on $(\hat{\Omega}, \mathcal{F}, \mu)$ with $\hat{\Omega}$ given in (2.3) and μ given in (2.9) (see underneath (6.5)). To estimate the l.h.s. of (6.151), note that for $E > 0$

$$\{\hat{\omega} : |S(\hat{\omega}, t)| > E\} \supseteq \{\hat{\omega} : |S(\hat{\omega}, t) \bmod I_k| > E\} \stackrel{(6.8)}{=} \{\hat{\omega} : |S_k(\hat{\omega}, t)| > E\}, \quad (6.152)$$

i.e. for any $k \in \mathbb{N}$ it follows that

$$\mu(|S(t)| > E) \stackrel{(6.152)}{\geq} \mu(|S_k(t)| > E). \quad (6.153)$$

Note that

$$\mu(|S_k(t)| > E) = \mathcal{P}_{k,t}((-\infty, -E] \cup [E, \infty)). \quad (6.154)$$

By (6.135) and Assertion 6.7 we have that

$$\begin{aligned} \lim_{t \rightarrow \infty} \mathcal{P}_{k,t}((-\infty, -E] \cup [E, \infty)) &= \mu \times \rho_{j_k}(f(Q, j) \in (-\infty, -E] \cup [E, \infty)) \\ &\stackrel{(6.136)}{=} \begin{cases} 1 - \frac{E}{2kL} & , \text{ if } E < 2kL \\ 0 & , \text{ if } E \geq 2kL. \end{cases} \end{aligned} \quad (6.155)$$

Let $E > 0$ be given. Let $k > \frac{E}{2L} := K_1(E)$, then by (6.155) for any $\varepsilon > 0$ there exists T_ε

such that for $t > T_\varepsilon$

$$\begin{aligned} & \left| \mathcal{P}_{k,t}((-\infty, -E] \cup [E, \infty)) - \left(1 - \frac{E}{2kL}\right) \right| < \varepsilon \\ \Leftrightarrow & -\varepsilon + 1 - \frac{E}{2kL} < \mathcal{P}_{k,t}((-\infty, -E] \cup [E, \infty)) < \varepsilon + 1 - \frac{E}{2kL}. \end{aligned} \quad (6.156)$$

Let $0 < \delta < 1$. Since

$$\lim_{k \rightarrow \infty} \frac{E}{2kL} = 0,$$

there exists $K_2(E)$ such that for $k > K_2(E)$

$$\frac{E}{2kL} < \frac{1 - \delta}{2}. \quad (6.157)$$

Then, we obtain by (6.156) with $\varepsilon = \frac{1-\delta}{2}$ that for $k > \max\{K_1(E), K_2(E)\}$ and $t > T_{\frac{1-\delta}{2}}$

$$\begin{aligned} \mathcal{P}_{k,t}((-\infty, -E] \cup [E, \infty)) & > -\frac{1-\delta}{2} + 1 - \frac{E}{2kL} \\ & \stackrel{(6.157)}{>} -\frac{1-\delta}{2} + 1 - \frac{1-\delta}{2} \\ & = \delta. \end{aligned} \quad (6.158)$$

From (6.158) we can follow that there exists $0 < \delta < 1$ such that for any $E > 0$ and $k > \max\{K_1(E), K_2(E)\}$

$$\sup_t \mathcal{P}_{k,t}((-\infty, -E] \cup [E, \infty)) > \delta. \quad (6.159)$$

By (6.153) (which holds for any k), (6.154) and (6.159) we obtain that there exists $0 < \delta < 1$ such that for any $E > 0$ and $k > \max\{K_1(E), K_2(E)\}$

$$\sup_t \mu(|S(t)| > E) \stackrel{(6.153)}{\geq} \sup_t \mathcal{P}_{k,t}((-\infty, -E] \cup [E, \infty)) \stackrel{(6.159)}{>} \delta.$$

Choosing

$$\hat{\varepsilon} = \delta$$

we obtain Lemma 6.7. □

By Lemma 6.7 we finally can prove Proposition 6.1.

Proof of Proposition 6.1. Let $C > 0$. We estimate the l.h.s. of (6.4). Recall that $S(t)$ (cf. (6.5)) differs from $\int_0^t U(s)ds$ in regard to $Q(0)$ (which is contained in $S(t)$) and in respect to $\sigma(0)$ ($S(t)$ is defined with $\sigma(0) = 1$, whereas $U(s)$ is the stationary process where $\sigma(0)$ is distributed according to $\rho_{\frac{1}{2}}$). To make use of Lemma 6.7 we write

$$\mu \times \rho_{\frac{1}{2}} \left(\left| \int_0^t U(s) ds \right| > C \right) \quad (6.160)$$

$$\begin{aligned} &= \mu \times \rho_{\frac{1}{2}} \left(\left\{ (\hat{\omega}, \sigma_0) : \left| \int_0^t \sigma(\sigma_0, \hat{\omega}, s) V(\hat{\omega}, s) ds \right| > C \right\} \right) \\ &= \mu \times \rho_{\frac{1}{2}} \left(\left\{ (\hat{\omega}, \sigma_0) : \left| \int_0^t \sigma(\sigma_0, \hat{\omega}, s) V(\hat{\omega}, s) ds \right| > C \right\} \cap \{\sigma_0 = 1\} \right) \\ &\quad + \mu \times \rho_{\frac{1}{2}} \left(\left\{ (\hat{\omega}, \sigma_0) : \left| \int_0^t \sigma(\sigma_0, \hat{\omega}, s) V(\hat{\omega}, s) ds \right| > C \right\} \cap \{\sigma_0 = -1\} \right) \\ &= 2\mu \times \rho_{\frac{1}{2}} \left(\left\{ (\hat{\omega}, \sigma_0) : \left| \int_0^t \sigma(\sigma_0, \hat{\omega}, s) V(\hat{\omega}, s) ds \right| > C \right\} \cap \{\sigma_0 = 1\} \right) \quad (6.161) \\ &= 2\mu \times \rho_{\frac{1}{2}} \left(\left\{ (\hat{\omega}, \sigma_0) : \left| \int_0^t \sigma(\sigma_0, \hat{\omega}, s) V(\hat{\omega}, s) ds \right| > C \right\} \Big| \{\sigma_0 = 1\} \right) \cdot \\ &\quad \cdot \mu \times \rho_{\frac{1}{2}}(\{\sigma_0 = 1\}) \end{aligned}$$

$$= \mu \left(\left\{ \hat{\omega} : \left| \int_0^t \sigma(\sigma_0 = 1, \hat{\omega}, s) V(\hat{\omega}, s) ds \right| > C \right\} \right). \quad (6.162)$$

Note that (6.161) follows, since

$$\int_0^t \sigma(\sigma_0 = 1, \hat{\omega}, s) V(\hat{\omega}, s) ds = - \int_0^t \sigma(\sigma_0 = -1, \hat{\omega}, s) V(\hat{\omega}, s) ds.$$

We now estimate (6.162). Since

$$\begin{aligned} &\mu \left(\left\{ \hat{\omega} : \left| \int_0^t \sigma(\sigma_0 = 1, \hat{\omega}, s) V(\hat{\omega}, s) ds \right| > C \right\} \right) = \\ &= \mu \left(\left\{ \hat{\omega} : \left| \int_0^t \sigma(\sigma_0 = 1, \hat{\omega}, s) V(\hat{\omega}, s) ds + Q(\hat{\omega}, 0) - Q(\hat{\omega}, 0) \right| > C \right\} \right) \end{aligned}$$

and

$$\begin{aligned} &\left\{ \hat{\omega} : \left| \int_0^t \sigma(\sigma_0 = 1, \hat{\omega}, s) V(\hat{\omega}, s) ds + Q(\hat{\omega}, 0) - Q(\hat{\omega}, 0) \right| > C \right\} \supseteq \\ &\supseteq \left\{ \hat{\omega} : \left| \int_0^t \sigma(\sigma_0 = 1, \hat{\omega}, s) V(\hat{\omega}, s) ds + Q(\hat{\omega}, 0) \right| - |Q(\hat{\omega}, 0)| > C \right\}, \quad (6.163) \end{aligned}$$

we estimate (6.162) by

$$\begin{aligned} &\mu \left(\left\{ \hat{\omega} : \left| \int_0^t \sigma(\sigma_0 = 1, \hat{\omega}, s) V(\hat{\omega}, s) ds \right| > C \right\} \right) \\ &\stackrel{(6.163)}{\geq} \mu \left(\left\{ \hat{\omega} : \left| \int_0^t \sigma(\sigma_0 = 1, \hat{\omega}, s) V(\hat{\omega}, s) ds + Q(\hat{\omega}, 0) \right| - |Q(\hat{\omega}, 0)| > C \right\} \right) \\ &\stackrel{(6.5)}{=} \mu(|S(t)| - |Q(0)| > C) \\ &= \mu(|S(t)| > C + |Q(0)|). \quad (6.164) \end{aligned}$$

Altogether we have by (6.160), (6.162), (6.164) and Lemma 6.7 for the l.h.s. of (6.4) and any $C > 0$ that

$$\sup_t \mu \times \rho_{\frac{1}{2}} \left(\left| \int_0^t U(s) ds \right| > C \right) \geq \sup_t \mu(|S(t)| > C + |Q(0)|) > \hat{\varepsilon}.$$

Choosing

$$\varepsilon = \hat{\varepsilon}$$

Proposition 6.1 follows. □

7 Discussion

In this chapter, we investigate whether the estimate of the rate given in (5.397) can further improved. Furthermore, we examine the approximate behavior of the estimate given in (5.400) for $L \rightarrow \infty$ or $M \rightarrow m$. We conclude the chapter with a discussion why the methods we used in the case $M > m$ fail for $M = m$.

7.1 Rate

7.1.1 Optimizing the rate estimate

The question rises whether the rate estimate given in (5.397) could be further improved. The second summand on the r.h.s of (5.397) prevents that the estimate has an exponential decay. Note that the estimate in (5.397) is based on the inequality of Corollary 5.2, i.e. on

$$\beta((n+1)t(\mathcal{G})) \leq 2 \left(\frac{\gamma(\mathcal{G})}{2} \right)^{n+1} + 8(n+1)\Pi(\mathcal{G}^c), \quad (7.1)$$

where $\mathcal{G} \subset \hat{\Omega}|_{\Lambda} \times \{-1, 1\}$, $t(\mathcal{G})$, $\gamma(\mathcal{G})$ fulfill Overlap-Lemma 5.2. The second summand in (5.397) is the result of the estimation of the second summand of the r.h.s. in (7.1).

First of all, note that \mathcal{G} has to be a proper subset of $\hat{\Omega}|_{\Lambda} \times \{-1, 1\}$, which is such that $\Pi(\mathcal{G}^c) = 0$ is not possible (see argumentation underneath Lemma 5.2).

In the derivation of (5.397), we have chosen $\mathcal{G} = G_{\bar{V}, \bar{N}}^c$ (cf. (5.10)) and \bar{V} and \bar{N} dependent on n such that

$$\Pi \left(G_{\bar{V}(n), \bar{N}(n)}^c \right) \leq \frac{C_{14}}{8} (n+1)^{-6}$$

(cf. (5.351)). It turns out that with this choice of $\bar{V}(n)$ and $\bar{N}(n)$, $\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)}^c)}{2}$ doesn't approach one too fast, and we obtain the estimate in (5.397).

The question whether the bound in (5.397) can be optimized or not is closely tied to whether \bar{V} and \bar{N} can be chosen dependent on n such that there exist $\tilde{N} \in \mathbb{N}$ and constants $C_{14}, a > 0$ such that for all $n > \tilde{N}$

$$\Pi \left(G_{\bar{V}(n), \bar{N}(n)}^c \right) \leq \frac{C_{14}}{8} \exp(-n^a), \quad (7.2)$$

where at the same time $\gamma(G_{\bar{V}(n), \bar{N}(n)})/2$ doesn't approach one too fast. By (5.359) and (5.368) we obtain that (7.2) is satisfied if

$$\bar{N}(n) \propto n^a$$

and

$$\bar{V}(n) \propto n^{\frac{a}{2}}.$$

This gives

$$\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)})}{2} \stackrel{(5.320)}{=} 1 - d_1 e^{-2d_2 n^a} \quad (7.3)$$

with some appropriate positive constants d_1, d_2 . Since $(1 - \frac{1}{\sqrt{n}})^n \rightarrow 0$ as $n \rightarrow \infty$, but $(1 - \frac{1}{n})^n \rightarrow e^{-1}$ as $n \rightarrow \infty$, a necessary condition to obtain a useful estimate having (7.1) in mind is that

$$d_1 e^{-2d_2 n^a} \geq \frac{1}{\sqrt{n}} \quad (7.4)$$

for n large enough, since

$$\left(\frac{\gamma(G_{\bar{V}(n), \bar{N}(n)})}{2} \right)^{n+1} = (1 - d_1 e^{-2d_2 n^a})^{n+1} \leq \left(1 - \frac{1}{\sqrt{n}} \right)^{n+1}$$

follows according to (7.3). However, (7.4) is equivalent to

$$n^a \leq \ln(\sqrt{n})$$

for n large enough, and since any root grows faster than the \ln -function, (7.4) can not be satisfied. Thus, there is no choice for $\bar{V}(n)$ and $\bar{N}(n)$ that satisfy (7.2) and such that $\frac{\gamma(\mathcal{G})}{2}$ doesn't approach 1 too fast, i.e. a bound for $\beta(i)$ with an exponential decay is not achievable.

7.1.2 Analyzing the estimate of the rate for $L \rightarrow \infty$ and $M \rightarrow m$

In this section, we analyze the bound of the rate given by (5.400) in order to gain insight whether the confinement of the molecule is necessary (see $L \rightarrow \infty$) and to obtain a good estimate for β if $M \rightarrow m$.

Here, the explicit description of the bound is given to highlight the dependency on L , M and m . We have by (5.400) with (5.394) and (5.395) for $i \in \mathbb{N}$ large enough that

$$\beta(i+1) \leq 2e^{-C_{15} i^{\frac{2}{5}}} + \left(32 \left(\frac{e^{-2L\rho}}{\sqrt{2\pi}} + (\sqrt{2\pi\mathcal{K}m})^{-1} \right) \right) i^{-4} \quad (7.5)$$

with

$$C_{15} \stackrel{(5.379)}{=} \frac{\delta}{4} \exp \left(- \frac{4\rho \left(\frac{24L}{B} + 3 \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \right)}{\sqrt{2\pi\mathcal{K}m}} \right), \quad (7.6)$$

where

$$D_b \stackrel{(5.25)}{=} \frac{4M^2}{m(M-m)}B \quad \text{and} \quad D_c \stackrel{(5.25)}{=} \frac{4M^2}{m(M-m)}B + \frac{2M-m}{2(M-m)}$$

and

$$\delta \stackrel{(5.312)}{=} g \cdot \exp \left(- \frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}} \right) \cdot C_{V_2} \cdot C_{\tau_2} \quad (7.7)$$

with $g, \bar{\tau}, C_{V_2}$ and C_{τ_2} given in (5.253), (5.242), (5.301), (5.302) if $M > 3m$, in (5.269), (5.268), (5.303), (5.304) if $M = 3m$, in (5.274), (5.273), (5.305), (5.306) if $3m > M > 2m$ and in (5.283), (5.282), (5.307), (5.308) if $2m \geq M > m$.

Analyzing the estimate of the rate for $L \rightarrow \infty$

First, we analyze the r.h.s. of (7.5) for $L \rightarrow \infty$, which means that the interval in which the molecule is confined, grows larger and larger. For that we express (7.6) in such a form that the dependence of L in (7.5) becomes more transparent. We begin with the factors in δ (cf. (7.7)). We write

$$g = c_1 \exp \left(- \frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}} \right) \quad (7.8)$$

with appropriate constant $c_1 > 0$. Note that $\bar{\tau}$ depends on L such that

$$\exp \left(- \frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}} \right) = \exp(-c_2L) \quad (7.9)$$

for some appropriate $c_2 > 0$, and let $c_4 > 0$ be an appropriate constant such that

$$C_{\tau_2} = c_4L. \quad (7.10)$$

Since C_{V_2} doesn't depend on L , we can express (7.7) as

$$\delta = c_1 C_{V_2} c_4 L \exp(-2c_2L) \quad (7.11)$$

with (7.8), (7.9) and (7.10). Note that the constants c_1, c_2, c_4 and C_{V_2} differ for the cases $M > 3m, M = 3m, 3m > M > 2m$ and $2m \geq M > m$.

Expressing the exponential function in (7.6) by

$$\exp\left(-\frac{4\rho\left(\frac{24L}{B} + 3\left(\rho\int_{D_b}^{D_c}vf(v)dv\right)^{-1}\right)}{\sqrt{2\pi\mathcal{K}m}}\right) = c_5 \exp(-c_6L) \quad (7.12)$$

with appropriate positive constants c_5 and c_6 , we obtain for (7.6) by (7.11) and (7.12) the expression

$$C_{15}(L) = \left(c_1C_{V_2}c_4c_5\frac{L}{4}\exp(-(2c_2 + c_6)L)\right). \quad (7.13)$$

Writing the second summand in (7.5) as

$$\left(32\left(\frac{e^{-2L\rho}}{\sqrt{2\pi}} + (\sqrt{2\pi\mathcal{K}m})^{-1}\right)\right)i^{-4} = c_7\exp(-c_8L)i^{-4} + c_9i^{-4} \quad (7.14)$$

with appropriate positive constants c_7 , c_8 and c_9 , we obtain together with (7.13) and (7.14) for (7.5) that

$$\begin{aligned} \beta(i+1) &\leq 2e^{-C_{15}i^{\frac{2}{5}}} + \left(32\left(\frac{e^{-2L\rho}}{\sqrt{2\pi}} + (\sqrt{2\pi\mathcal{K}m})^{-1}\right)\right)i^{-4} = \\ &= 2\exp\left(-\left(c_1C_{V_2}c_4c_5\frac{L}{4}\exp(-(2c_2 + c_6)L)\right)i^{\frac{2}{5}}\right) + c_7\exp(-c_8L)i^{-4} + c_9i^{-4} \\ &\rightarrow 2 + c_9i^{-4} \end{aligned} \quad (7.15)$$

as $L \rightarrow \infty$, i.e. the bound for β becomes unfeasible, since we cannot follow from (7.15) that $\beta(t)$ is integrable.

Heuristically, the bound becomes unfeasible for $L \rightarrow \infty$, since the derivation of the bound is based on the fact that the time when overlap occurs is finite (see Overlap-Lemma 5.2). To establish overlap, we first pushed atoms in Λ to obtain the molecule alone in the interval. The larger Λ , i.e. the larger L , the longer it takes to obtain a state, where the molecule is alone in the interval. Hence, if $L \rightarrow \infty$, the time where overlap occurs is not finite anymore and the estimate becomes unfeasible.

Analyzing the estimate of the rate for $M \rightarrow m$

Now we analyze the r.h.s. of (7.5) for $M \rightarrow m$. Since only M near to m is of interest, we use $g, \bar{\tau}, C_{V_2}$ and C_{τ_2} as given in (5.283), (5.282), (5.307) and (5.308), since these are the choices for $g, \bar{\tau}, C_{V_2}$ and C_{τ_2} if $m < M \leq 2m$.

As $M \rightarrow m$ we have that

$$\bar{\tau} \stackrel{(5.282)}{=} \frac{2L}{C} + \frac{8LM + m}{B(M - m)} \rightarrow \infty. \quad (7.16)$$

This gives that

$$g \stackrel{(5.283)}{=} \rho \sqrt{\frac{\mathcal{K}m}{2\pi}} e^{-\frac{\kappa m}{2} \left(\frac{1}{2m} \frac{9M^2}{M+m} B + \frac{M-m}{2m} \frac{B}{4} \right)^2} \left(\frac{M+m}{2m} \right)^2 \frac{B}{4} \frac{M-m}{M+m} \frac{M+7m}{2(M+3m)} e^{-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}} \rightarrow 0. \quad (7.17)$$

Since for $M \rightarrow m$

$$C_{V_2} \stackrel{(5.307)}{=} \frac{M-m}{2(M+3m)} \frac{M-m}{M+m} \frac{B}{4} \rightarrow 0 \quad (7.18)$$

and C_{τ_2} is a constant independent of M , we obtain with (7.16), (7.17) and (7.18) for (7.7) that

$$\delta = g \cdot \exp\left(-\frac{2\bar{\tau}\rho}{\sqrt{2\pi\mathcal{K}m}}\right) \cdot C_{V_2} \cdot C_{\tau_2} \rightarrow 0 \quad (7.19)$$

as $M \rightarrow m$.

To analyze the behavior of the exponential function in (7.6), note that

$$\int_a^b v f(v) dv = \frac{1}{\sqrt{2\pi\mathcal{K}m}} \left(e^{-\frac{\kappa m}{2} a^2} - e^{-\frac{\kappa m}{2} b^2} \right).$$

With that and introducing the constant c_{10} we have that

$$\begin{aligned} & \exp\left(-\frac{4\rho \left(\frac{24L}{B} + 3 \left(\rho \int_{D_b}^{D_c} v f(v) dv \right)^{-1} \right)}{\sqrt{2\pi\mathcal{K}m}}\right) \\ &= \exp\left(-\frac{4\rho \frac{24L}{B}}{\sqrt{2\pi\mathcal{K}m}}\right) \exp\left(-\frac{12}{\sqrt{2\pi\mathcal{K}m} \int_{D_b}^{D_c} v f(v) dv}\right) \\ &= c_{10} \exp\left(-\frac{12}{e^{-\frac{\kappa m}{2} \left(\frac{4M^2}{m(M-m)} B \right)^2} - e^{-\frac{\kappa m}{2} \left(\frac{4M^2}{m(M-m)} B + \frac{2M-m}{2(M-m)} B \right)^2}}\right) \\ &= c_{10} \exp\left(-\frac{12}{e^{-\frac{\kappa m}{2} \left(\frac{4M^2}{m(M-m)} B \right)^2} \left(1 - e^{-\frac{\kappa m}{2} \left(2 \frac{4M^2}{m(M-m)} B \frac{2M-m}{2(M-m)} B + \left(\frac{2M-m}{2(M-m)} B \right)^2 \right)} \right)}\right) \\ &= c_{10} \exp\left(-\frac{12}{e^{-\frac{\kappa m}{2} \left(\frac{4M^2}{m(M-m)} B \right)^2} \left(1 - e^{-\frac{\kappa m}{2} \frac{(2M-m)(16M^2 + (M-m)m)}{4m(M-m)^2} B^2} \right)}\right) \\ &\rightarrow 0 \end{aligned} \quad (7.20)$$

as $M \rightarrow m$. By (7.19) and (7.20) we obtain for (7.6) that

$$C_{15} \rightarrow 0$$

as $M \rightarrow m$. This gives for (7.5) that

$$\begin{aligned} \beta(i+1) &\leq 2e^{-C_{15}i^{\frac{2}{5}}} + \left(32 \left(\frac{e^{-2L\rho}}{\sqrt{2\pi}} + (\sqrt{2\pi\mathcal{K}m})^{-1} \right) \right) i^{-4} \\ &\rightarrow 2 + \left(32 \left(\frac{e^{-2L\rho}}{\sqrt{2\pi}} + (\sqrt{2\pi\mathcal{K}m})^{-1} \right) \right) i^{-4} \end{aligned}$$

as $M \rightarrow m$. Hence, for $M \rightarrow m$ the r.h.s. of (7.5) becomes an unfeasible bound for β . Heuristically, the estimate becomes unfeasible, because, like in the previous case where $L \rightarrow \infty$, the time where overlap occurs, approaches ∞ if $M \rightarrow m$ (cf. Overlap-Lemma 5.2). However, having the proof of the Overlap-Lemma 5.2 in mind, it becomes clear that the “good set” \mathcal{G} should be chosen anyhow differently in the equal mass case. We discuss the proof for $M = m$ with a different set \mathcal{G} in the following section.

7.2 Why the methods we used for $M > m$ fail for $M = m$

Recall that the first part of our main result, Theorem 2.1 excl. $D > 0$, follows by Proposition 5.1. Proposition 5.1 can be proven by establishing overlap of Π_y^t and Π for y in a “good” set \mathcal{G} (see Overlap-Lemma 5.2). By the existence of an overlap at time $t(\mathcal{G})$ one obtains that

$$\beta((n+1)t(\mathcal{G})) \leq 2 \left(\frac{\gamma(\mathcal{G})}{2} \right)^{n+1} + 8(n+1)\Pi(\mathcal{G}^c)$$

(cf. Corollary 5.2). For $M > m$ we chose $\mathcal{G} = G_{\bar{V}, \bar{N}}$ as given in (5.10). Then, we chose $G_{\bar{V}, \bar{N}}$ as depending on time and showed that $\Pi(G_{\bar{V}, \bar{N}}^c)$ tends to zero fast enough as $t \rightarrow \infty$, where at the same time $\gamma(G_{\bar{V}, \bar{N}})/2$ doesn't tend too fast to one.

If $M = m$ we have to choose another good set \mathcal{G} : The problematic starting states are now these where at least one particle in Λ has velocity 0. Since the particles exchange velocities, there will be at any time a particle with $v = 0$ resp. $V = 0$. It's impossible to reach a state, where the molecule is alone in the interval with velocity $V > 0$. On the other hand, states where all particles in the interval have non-zero velocities will never reach a state where the molecule is alone in Λ with $V = 0$. Hence, if $M = m$ the states where at least one particle in the interval has velocity zero need to be excluded from \mathcal{G} , otherwise no overlap set can be established. Denote by $G_{\underline{V}} \subset \hat{\Omega} \times \{-1, 1\}$ the set of configurations where no particle has speed lower than $\underline{V} > 0$, i.e. with ease of notation

$$G_{\underline{V}} := \{|v|, |V| > \underline{V}\}.$$

One can show that $G_{\underline{V}}$ fulfills Overlap-Lemma 5.2, which means that we obtain by Corollary 5.2 that

$$\beta((n+1)t(\underline{V})) \leq 2 \left(\frac{\gamma(\underline{V})}{2} \right)^{(n+1)} + 8(n+1)\Pi(G_{\underline{V}}^c)$$

where $G_{\underline{V}}^c$ is the complement of $G_{\underline{V}}$, i.e. the set of all configurations where at least one particle in Λ has speed less than \underline{V} . To show Proposition 5.1, we have to choose $G_{\underline{V}}$, i.e. \underline{V} , dependent on n such that on the one hand

$$\Pi(G_{\underline{V}(n)}^c) < (n+1)^{-K} \tag{7.21}$$

for n large enough and an appropriate $K > 2$, but on the other hand

$$\frac{\gamma(\underline{V}(n))}{2} \tag{7.22}$$

doesn't tend too fast to one with $n \rightarrow \infty$. (7.21) holds if $\underline{V}(n)$ approaches zero fast enough, on the other hand (7.22) requires that $\underline{V}(n)$ doesn't tend too fast to zero. Since the velocities are distributed according to the Maxwell distribution, i.e. small velocities are likely, $\underline{V}(n)$ has to tend to zero quite fast to obtain (7.21). As it turns out, there is no choice of $\underline{V}(n)$, such that (7.21) and (7.22) can be fulfilled.

The difference to the case where $M > m$ is the following. If $M > m$, $\bar{V}(n)$ and $\bar{N}(n)$ shouldn't approach ∞ too fast, such that $\gamma(G_{\bar{V}, \bar{N}})/2$ doesn't tend too fast to one, and on the other hand $\bar{V}(n)$ and $\bar{N}(n)$ have to grow fast enough, such that $\Pi(G_{\bar{V}, \bar{N}}^c) < (n+1)^{-K}$. Since the Maxwell distribution helps that $\Pi(G_{\bar{V}, \bar{N}}^c)$ is small (many particles in Λ are unlikely, such as very fast atoms), one can find $\bar{V}(n), \bar{N}(n)$ such that both conditions are fulfilled.

8 Outlook

8.1 A model without confinement of the molecule

We would like to point out an observation, the meaning of which should be further scrutinized. We can set L dependent on time such that we keep a good mixing rate. This is our point towards another Markovian model, which (i) is perhaps closer to the physical model of a mass moving in an ideal gas in one dimension and (ii) allows showing diffusion. For this we choose L dependent on time $i \in \mathbb{N}$ such that $L(i) \rightarrow \infty$ with $i \rightarrow \infty$. To keep (7.5) a good estimate for $\beta(i+1)$, it is necessary that for the first summand of the r.h.s. of (7.5) for i large enough

$$\begin{aligned} e^{-C_{15}(L(i))i^{\frac{2}{5}}} &< \frac{1}{i^2} \\ \Leftrightarrow -C_{15}(L(i))i^{\frac{2}{5}} &< -\ln(i^2) \\ \Leftrightarrow C_{15}(L(i)) &> \ln(i^2)i^{-\frac{2}{5}}. \end{aligned} \tag{8.1}$$

with C_{15} given in (7.6). Inequality (8.1) is satisfied if $L(i)$ is for example such that for i large enough

$$C_{15}(L(i)) > i^{-\frac{3}{10}}. \tag{8.2}$$

Since

$$C_{15}(L(i)) \stackrel{(7.13)}{=} d_1 L(i) \exp(-d_2 L(i))$$

with

$$d_1 := \frac{1}{4}c_1 C_{V_2} c_4 c_5$$

and

$$d_2 := 2c_2 + c_6, \tag{8.3}$$

(8.2) is equivalent to

$$\begin{aligned} C_{15}(L(i)) &> i^{-\frac{3}{10}} \\ \Leftrightarrow d_1 L(i) \exp(-d_2 L(i)) &> i^{-\frac{3}{10}} \end{aligned}$$

$$\begin{aligned}
&\Leftrightarrow \exp(\ln(d_1 L(i)) - d_2 L(i)) > i^{-\frac{3}{10}} \\
&\Leftrightarrow \ln(d_1 L(i)) - d_2 L(i) > -\frac{3}{10} \ln(i) \\
&\Leftrightarrow d_2 L(i) - \ln(d_1 L(i)) < \frac{3}{10} \ln(i).
\end{aligned} \tag{8.4}$$

If we choose for example

$$L(i) = \frac{3}{10d_2} \ln(i) \tag{8.5}$$

we obtain (8.2) for i large enough, since with the choice (8.5) inequality (8.4) is satisfied for i large enough.

Altogether, we obtain for (7.5) by (8.2) and (8.5) that

$$\begin{aligned}
\beta(i+1) &\leq 2e^{-C_{15}i^{\frac{2}{5}}} + \left(32 \left(\frac{e^{-2L(i)\rho}}{\sqrt{2\pi}} + (\sqrt{2\pi\mathcal{K}m})^{-1} \right) \right) i^{-4} \\
&< 2e^{-i^{-\frac{3}{10}}i^{\frac{2}{5}}} + \left(32 \left(\frac{e^{-\frac{6\rho}{10d_2} \ln(i)}}{\sqrt{2\pi}} + (\sqrt{2\pi\mathcal{K}m})^{-1} \right) \right) i^{-4} \\
&= 2e^{-i^{\frac{1}{10}}} + \frac{32}{\sqrt{2\pi}} i^{-\left(\frac{6\rho}{10d_2}+4\right)} + \frac{32}{\sqrt{2\pi\mathcal{K}m}} i^{-4}
\end{aligned}$$

with the positive constant d_2 given in (8.3).

8.2 A multidimensional model

We expect that the method employed for the presented model can also be applied to provide a fCLT for the multidimensional case. Consider the following model: The molecule, with radius R , confined in a convex compact domain and is surrounded by an ideal gas of point particles, which are not directly affected by the barrier. Ergodic properties of this model were investigated in [ET90]. General ideas how to prove diffusive behavior for

$$Q(t) = \int_0^t |V(s)| ds$$

in the usual scaling in this multidimensional model are outlined in [ET92] based on a theorem of [Ore59]. They mentioned a difficulty which also occurs when proving diffusive behavior for

$$R(t) = \int_0^t \sigma(s)V(s) ds$$

in the usual scaling with the methods we used in the presented one dimensional model: Consider for simplicity the molecule is confined in a ball. Having our proof for the one dimensional model in mind, to obtain overlap, it is useful to show that the system reaches a state where the molecule is alone in the ball with a certain range of speed with positive probability. Once the system is in such a state, one can control the molecule by sending in atoms to establish overlap. To obtain a state where the molecule is alone in the ball, we control the molecule by sending in other atoms, such that the molecule kicks out all atoms which are in the ball. But atoms which are close to the boundary cannot be kicked out: Before the molecule collides with these to kick them out, the molecule is reflected at the boundary. Hence, states where very slow atoms are near to the boundary are problematic states. This problem should be solvable by reducing \mathcal{G} , the set of good starting states for which overlap shall be established, by states which include these problematic situations. Using a similar procedure as in the proof of Lemma 1 of [ET90], where atoms are send in to obtain a state where the molecule is alone in the domain, one should be able to obtain a Lemma analogue to Lemma 5.6 in Chapter 5. The analogue to the Overlap-Lemma 5.2 should follow easily.

Therefore, we expect that the methods presented within the scope of this work can be applied to the multidimensional model without any major difficulties.

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