On the zero mass limit of tagged particle diffusion in the 1-d Rayleigh-gas

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Dedicated to Domokos Szász on his 65th birthday

Abstract

We consider the $M \to 0$ limit for tagged particle diffusion in a 1-dimensional Rayleigh-gas, studied originaly by Sinai and Soloveichik [16], and by Szász and Tóth [21], respectively. In this limit we derive a new type of model for tagged particle diffusion, for which the two central particles, in addition to elastic collisions with the rest of the gas, interact with Calogero-Moser-Sutherland (i.e. inverse quadratic) potential. Computer simulations on this new model reproduce exactly the numerical value of the limiting variance obtained by Boldrighini, Frigio and Tognetti in [4].

1 Introduction

The problem of deriving relevant information on the diffusive scaling limit of tagged particle motion (i.e. self-diffusion) from microscopic principles has undoubtedly been at the heart of mathematically rigorous statistical physics of time dependent phenomena, at least since Einstein's groundbreaking work. Mathematically rigorous investigation of tagged particle diffusion in systems of particles governed by deterministic (Hamiltonian) dynamics is notoriously difficult, even in one dimensional models. After remarkable advances made through the late 1980-s (see Section 3 below and references cited there), in the last twenty years there has seemed to be less intense activity in the field. This is certainly due to the difficulty of these problems and the lack of technical tools to attack them.

In the present note we make a small but (hopefully) not irrelevant contribution to the subject. We investigate the $M \to 0$ small mass limit of the tagged particle diffusion in the so-called 1-dimensional Rayleigh-gas. This system consists of an infinitely extended one-dimensional gas of point-like particles of mass 1 and one single tagged particle of mass M immersed in it. The particles perform uniform motion and interact through elastic collisions. The system is distributed according to the equilibrium Gibbs measure. This means independent exponentially distributed inter-particle distances and independent normally distributed velocities with mean zero and inverse mass variances, so that the kinetic energy is equidistributed. It is a fact that the dynamics of the infinitely extended system are almost surely well defined under this stationary measure. In other words no multiple collisions and no accumulations of infinitely many particles in finite time occur. Randomness comes into the problem only through the thermal equilibrium of the initial condition, otherwise the dynamical evolution is deterministic. The central question is to understand the diffusive scaling limit of the trajectory of the tagged particle: $A^{-1/2}Q_{At}$, as $A \to \infty$. There exist a number of deep and interesting results related to this problem that will be briefly surveyed in Section 3.

In the present note we investigate the limit when $M \to 0$. We prove that in this limit the system becomes equivalent to another, new model of tagged particle motion. This new model differs from the one described above in two aspects. On the one hand, instead of one central particle of different mass, all particles have the same (unit) mass. On the other hand, however, there are two distinguished central particles which, in additon to elastic collisions with the rest of the gas, also interact via a Calogero-Moser-Sutherland-type repulsive potential with a random strength parameter. To avoid confusion we emphasize that elastic collisions play an improtant role in the dynamics. In particular, when considering the motion of the two central particles, only *piecewise* integrable behaviour can be observed: when colliding with the rest of the gas, the central two-particle system switches instantaneously from one trajectory of the pair-potential interaction to another. On further details see Section 2.2.2 and Figure 1.

Another improtant feature of our new model is that the strength parameter of the repulsive potential is random, more precisely, it is determined by the (random) initial conditions. This fact provides explanation to some phenomena observed in earlier computer simulations on the Rayleigh-gas, in particular to the instability observed for small values of M.

We also present numerical simulations on this new model. Our simulation results reproduce very accurately the numerical value of the tagged particle's limiting variance in the Rayleigh-gas, in the $M \to 0$ limit, which was obtained in [4]. We claim that our result not only reproduces, from a completely different approach, the numerical value, but also gives a theoretical explanation of the phenomenon.

It is interesting to note that the same type of potential interaction has been observed to occur in a different, though related context: the one-dimensional piston problem studied by Sinai ([15]), by Sinai and Neishtadt ([13]) and by Wright ([24]), respectively. This is not a coincidence, the appearence of the inverse quadratic potential is a consequence of averaging for the fast degrees of freedom in these one dimensional systems, see the calculations in the above mentioned articles and in Section 4 of our paper.

The rest of the paper is organized as follows: In Section 2 we define the models of interacting particle systems considered, their stationary Gibbs measures and the stochastic processes whose diffusive asymptotics are later analysed. In Section 3 we briefly survey the existing earlier results (rigorously proved and numerical alike) on tagged particle diffusion in the 1-d Rayleigh-gas. In Section 4 we properly state and prove the theorem which states that in the $M \to 0$ limit, the 1-d dynamics of the Rayleigh-gas with tagged particle of mass M converges (trajectory-wise, in a natural topology) to the dynamics of the above mentioned model: a 1-d gas of particles with equal masses colliding elastically, and, furthermore, a Calogero-Moser-Sutherland interaction between the two central particles. Finally, in Section 5 we present our new numerical results referring to this new type of interacting particle system. We should emphasize here that our numerical results are performed for a genuinely new type of model, and thus they are not just accurate reproductions of older computer experiments. One of the main points of this paper is that these genuinely new numerical results are both in accurate agreement with the results of Boldrighini, Frigio, Tognetti [4], and give independent enhancement *and theoretical explanation* to them.

2 Models: state space, dynamics, stationary measures

In this section we describe the models considered throughout the paper. In section 2.1 we present a formal definition of the state spaces and the natural measures on them. Section 2.2, which gives a more verbal description of the time evolution in our dynamical systems, clarifies that these models indeed correspond to the one dimensional gases mentioned in the Introduction.

2.1 State spaces and stationary Gibbs measures

Let

$$\Omega^{\pm} := \{\omega^{\pm} = (x_{\pm i}, v_{\pm i})_{i=1}^{\infty} : (x_{\pm i}, v_{\pm i}) \in \mathbb{R}_{\pm} \times \mathbb{R}, \quad x_{\pm 1} = 0, \quad \pm(x_{\pm(i+1)} - x_{\pm i}) \geq 0\}.$$

With a slight abuse of notation and terminology we sometimes don't distinguish between $\omega^{\pm}$ and the (unordered) set of points $\{(x_{\pm i}, v_{\pm i}) : i = 1, 2, \dots\} \subset \mathbb{R}_{\pm} \times \mathbb{R}$. We endow the spaces $\Omega^{\pm}$ with the topology defined by pointwise convergence: $\omega_n^{\pm} \to \omega^{\pm}$ iff $(x_{\pm i}, v_{\pm i})_n \to (x_{\pm i}, v_{\pm i})$, for all $i = 1, 2, \dots$. This is a metrizable topology and makes the $\Omega^{\pm}$ complete and separable (i.e. Polish) spaces.

We denote by $\mu^\pm$ the following probability measures over $\Omega^\pm$, respectively. Under $\mu^\pm$ the random variables $\xi_{\pm i} := \pm\big(x_{\pm(i+1)} - x_{\pm i}\big)$, $\eta_{\pm j} := v_{\pm j}$, $i, j = 1, 2, \dots$, are completely independent, with exponential, respectively, normal distributions:

$$\mathbf{P}\big(\xi_{\pm i} \in (x, x + \mathrm{d}x)\big) = 1\!\!1_{\{x \geq 0\}} e^{-x}\,\mathrm{d}x, \quad \mathbf{P}\big(\eta_{\pm j} \in (v, v + \mathrm{d}v)\big) = \frac{1}{\sqrt{2\pi}} e^{-v^2/2}\,\mathrm{d}v.$$

We shall consider two different types of particle systems in this paper. Their state spaces will be

$$\begin{aligned} \Omega^{I} &:= \{(\omega^+, \omega^-, z, u, V) : \omega^\pm \in \Omega^\pm, \quad z \in \mathbb{R}_+, \quad u \in [-1, 1], \quad V \in \mathbb{R}\}, \\ \Omega^{II} &:= \{(\omega^+, \omega^-, z) : \omega^\pm \in \Omega^\pm, \quad z \in \mathbb{R}_+\}. \end{aligned}$$

We also define the natural projection between these spaces:

$$\Pi : \Omega^{I} \to \Omega^{II}, \qquad \Pi(\omega^+, \omega^-, z, u, V) := (\omega^+, \omega^-, z).$$

Remark. The physical meaning of the coordinates $z; u; \dots$ etc. in the relevant dynamical models are discussed in the next subsection.

In order to define the relevant probability measures on the state spaces Ω^{I} and Ω^{II}, we first introduce some notation. Let the random variables W and ζ be independent with W distributed as a standard Gaussian, and ζ distributed as a standard $\Gamma(2)$. Let $\gamma_2(z)$ be the density of the distribution of ζ, $\varrho(c)$ the density of the distribution of $|W\zeta|$, and $\varphi_c(z)$ the density of the conditional distribution of ζ, given $|W\zeta| = c$:

$$\begin{aligned} \gamma_2(z) &:= z e^{-z}, \\ \varrho(c) &:= \sqrt{\frac{2}{\pi}} \int_0^\infty \exp\{-z - \frac{c^2}{2z^2}\}\,\mathrm{d}z, \\ \varphi_c(z) &:= \frac{1}{\varrho(c)} \sqrt{\frac{2}{\pi}} \exp\{-z - \frac{c^2}{2z^2}\}. \end{aligned}$$

Clearly,

$$\gamma_2(z) = \int_0^\infty \varphi_c(z) \varrho(c)\,\mathrm{d}c.$$

The probability measures considered on the state spaces Ω^{I} and Ω^{II} are $\mu^{I,M}$, defined on Ω^{I}, which depends on the positive parameter M, $\mu^{II,c}$, defined on Ω^{II}, which depends on the positive parameter c, and finally μ^{II}, also defined on Ω^{II}, which is a mixture of the measures $\mu^{II,c}$:

$$\mu^{I,M}(\mathrm{d}\omega^{I}) := \mu^+(\mathrm{d}\omega^+) \times \mu^-(\mathrm{d}\omega^-) \times \gamma_2(z)\,\mathrm{d}z \times \frac{1}{2}\mathrm{d}u \times \sqrt{\frac{M}{2\pi}} e^{-MV^2/2}\,\mathrm{d}V, \tag{1}$$

$$\mu^{II,c}(\mathrm{d}\omega^{II}) := \mu^+(\mathrm{d}\omega^+) \times \mu^-(\mathrm{d}\omega^-) \times \varphi_c(z)\,\mathrm{d}z, \tag{2}$$

$$\begin{aligned} \mu^{II}(\mathrm{d}\omega^{II}) &:= \mu^+(\mathrm{d}\omega^+) \times \mu^-(\mathrm{d}\omega^-) \times \gamma_2(z)\,\mathrm{d}z \\ &= \int_0^\infty \mu^{II,c}(\mathrm{d}\omega^{II}) \varrho(c)\,\mathrm{d}c. \end{aligned} \tag{3}$$

The measures $\mu^{I,M}$ and $\mu^{II,c}$ will be the natural Gibbs measures corresponding to the dynamics of our systems, to be defined in the next subsection.

2.2 Dynamics

We define the dynamics of the systems considered verbally, rather than writing formulas. The two types of dynamics considered will be called *of type I* and of *of type II*. Their state spaces will be Ω^I and Ω^{II}, respectively. These will actually be two families of dynamics parametrized by the fixed parameters $M > 0$, $c > 0$, respectively.

2.2.1 Dynamics of type I:

For precise formal definitions and basic facts about these dynamics, see [16], [21], [22]. The system consists of particles indexed $\dots, -2, -1, 0, +1, +2, \dots$. The system is observed from the tagged particle of index 0. The tagged particle has mass M, and the other particles have unit mass. Positions and velocities of the particles in the system are encoded in $(\omega^+, \omega^-, z, u, V)$ as follows: V is the velocity of the tagged particle, $x_{\pm i} \pm z(1 \pm u)/2$ and $v_{\pm i}$ are the position and the velocity, respectively, of the particle of index $\pm i$, $i = 1, 2, \dots$. The untagged gas particles perform uniform motion on the line and don't interact between themselves. When two of them meet and cross each other's trajectory, they exchange their indices. The tagged particle, while isolated from the others, also performs uniform motion and collides elastically at encounters with an untagged gas particle. At these collisions the outgoing velocities $V^{\text{out}}, v^{\text{out}}$ are determined by the incoming velocities $V^{\text{in}}, v^{\text{in}}$ as follows:

$$V^{\text{out}} = \frac{M-1}{M+1} V^{\text{in}} + \frac{2}{M+1} v^{\text{in}}, \qquad v^{\text{out}} = \frac{2M}{M+1} V^{\text{in}} - \frac{M-1}{M+1} v^{\text{in}}. \tag{4}$$

Note that the untagged gas particles never exchange their order with the tagged particle, and the index $\pm i$ of a particle denotes its actual relative order with respect to the tagged particle.

The measure $\mu^{I,M}$ defined in (1) is the Gibbs measure for these dynamics, invariant for the system as seen from the tagged particle. It is a fact (see [16], [21], [22]) that these dynamics are $\mu^{I,M}$-a.s. well defined: starting the system distributed according to $\mu^{I,M}$, with probability 1 no multiple collisions will occur and the system remains locally finite indefinitely. We denote by $\mathcal{S}_t^{I,M}$ the measure preserving flow on $(\Omega^I, \mu^{I,M})$ defined by this dynamics.

The velocity and displacement processes of the tagged particle are

$$\begin{aligned} V_t^{I,M} &= V_t^{I,M}(\omega^I) := V(\mathcal{S}_t^{I,M}\omega^I) \\ Q_t^{I,M} &= Q_t^{I,M}(\omega^I) := \int_0^t V_s^{I,M}(\omega^I)\, \mathrm{d}s. \end{aligned}$$

In Section 4 it will be more convenient to describe the dynamics from a fixed exterior point of observation. The absolute locations of the gas particles in the system as seen from such a fixed exterior frame of reference are

$$y_{\pm i}(t) := Q_t^{I,M} + x_{\pm i}(t), \quad \text{where} \quad x_{\pm i}(t) := x_{\pm i}(\mathcal{S}_t^{I,M}\omega^I), \qquad i = 1, 2, \dots. \tag{5}$$

We also introduce the variables

$$\widetilde{V}_t^{I,M} = \widetilde{V}_t^{I,M}(\omega^I) := \frac{1}{2}\Big(v_{-1}(\mathcal{S}_t^{I,M}\omega^I) + v_{+1}(\mathcal{S}_t^{I,M}\omega^I)\Big)$$
$$\widetilde{Q}_t^{I,M} = \widetilde{Q}_t^{I,M}(\omega^I) := \int_0^t \widetilde{V}_s^{I,M}(\omega^I)\,\mathrm{d}s.$$

These are the velocity and position processes of the centre of mass of the particles directly to the right and to the left of the tagged particle. We need the position process $\widetilde{Q}_t^{I,M}$ for later comparison with a similar process defined for the dynamics of type II in the next paragraph. Observe that the random process $t \mapsto \big(Q_t^{I,M} - \widetilde{Q}_t^{I,M}\big)$ is stationary and thus tight, uniformly for $t > 0$. As a consequence, $\big(Q_t^{I,M}/\sqrt{t} - \widetilde{Q}_t^{I,M}/\sqrt{t}\big) \to 0$ in $\mu^{I,M}$-probability (actually $\mu^{I,M}$-a.s.) as $t \to \infty$.

2.2.2 Dynamics of type *II*:

The system consists of particles of unit mass indexed $\dots, -2, -1, +1, +2, \dots$. Note that there is no particle of index 0 in this system. The system is observed from the centre of mass of particles of index $+1$ and -1, which we call the central observation point. Positions and velocities of the particles in the system are encoded in (ω^+, ω^-, z) as follows: $x_{\pm i} \pm z/2$ and $v_{\pm i}$ are the position relative to the central observation point and the velocity, respectively, of the particle of index $\pm i$, $i = 1, 2, \dots$. Clearly, z denotes the distance between the two central particles of index $+1$ and -1. Particles move uniformly on the line except for the two central particles of index $+1$ and -1. *Between collisions with the rest of the gas*, the motion of the two central particles is governed by interaction via the inverse quadratic pair potential $U(z)$, or equivalently via the repelling force $F(z)$:

$$U(z) = \frac{c^2}{2z^2}, \qquad F(z) = \frac{c^2}{z^3}. \tag{6}$$

Here $c^2 > 0$ is a fixed parameter while z, as mentioned above, is the distance between the two central particles. When two gas particles meet, they exchange their index. In particular, when a particle of index ± 1 collides with a particle of a different index, its velocity changes instantaneously. As a result of this instantaneous effect, the central two-particle system, which follows a trajectory corresponding to the integrable pair-potential (6) between collisions, jumps from one such trajectory to another when colliding with the rest of the gas. This may be regarded as an instantantanous change in the initial conditions of the two-particle system. In case two non-central particles collide, the convention that they exchange their index simply reflects that they cross each other's trajectory. Note, furthermore, that due to the strongly repulsive interaction between the two central particles, these two will never meet. Thus particles will never change the sign of their index. The index $\pm i$ of a particle always denotes its actual relative order with respect to the central observation point. See Figure 1 for a simulated trajectory of these dynamics.

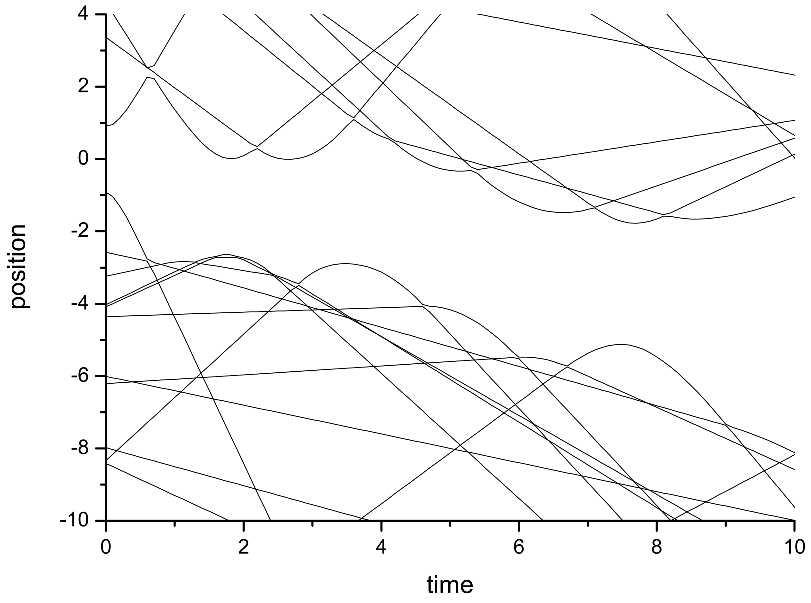

Figure 1: Trajectory of the particles with indices $|i| \leq 30$ for the time interval $0 < t < 10$ in the Type II dynamics, with $c = 10$.

Remark. In the literature of completely integrable Hamiltonian systems the pair potential (6) is usually called the Calogero-Moser-Sutherland interaction and leads to one of the most notorious completely integrable systems on the one dimensional line $\mathbb{R}^1$, see [5], [11] and [20] for the original publications. We would like to stress, however, that our system is not integrable, due to the presence of the further gas particles (cf. the change of initial conditions at collisions described above).

The measure $\mu^{II,c}$ defined in (2) is the Gibbs measure for these dynamics, invariant for the system as seen from the centre of mass of the two central particles. It is again a fact that these dynamics are $\mu^{II,c}$-a.s. well defined. We denote by $\mathcal{S}_t^{II,c}$ the measure preserving flow defined by these dynamics on $(\Omega^{II}, \mu^{II,c})$.

The velocity and displacement process of the point of observation is

$$V_t^{II,c} = V_t^{II,c}(\omega^{II}) := \frac{1}{2}\big(v_{-1}(\mathcal{S}_t^{II,c}\omega^{II}) + v_{+1}(\mathcal{S}_t^{II,c}\omega^{II})\big)$$

$$Q_t^{II,c} = Q_t^{II,c}(\omega^{II}) := \int_0^t V_s^{II,c}(\omega^{II})\,\mathrm{d}s.$$

Again, absolute locations of the gas particles in the system as seen from a fixed exterior frame of reference are expressed similarly to (5).

2.2.3 Stochastic processes considered

In this paper we consider the following *stochastic processes*:

$$
\begin{aligned}
Q_t^{I,M} &= Q_t^{I,M}(\omega^I), \quad \text{with random } \omega^I \text{ distributed according to} \quad \mathrm{d}\mu^{I,M},\\
\widetilde{Q}_t^{I,M} &= \widetilde{Q}_t^{I,M}(\omega^I), \quad \text{with random } \omega^I \text{ distributed according to} \quad \mathrm{d}\mu^{I,M},\\
Q_t^{II,c} &= Q_t^{II,c}(\omega^{II}), \quad \text{with random } \omega^{II} \text{ distributed according to} \quad \mathrm{d}\mu^{II,c},\\
Q_t^{II} &= Q_t^{II,c}(\omega^{II}), \quad \text{with random } (\omega^{II}, c) \text{ distributed according to} \quad \mathrm{d}\mu^{II,c}\varrho(c)\,\mathrm{d}c,\\
&= Q_t^{II,c}, \quad \text{with random } c \text{ distributed according to} \quad \varrho(c)\,\mathrm{d}c.
\end{aligned}
$$

This means that the process Q_t^{II} is a $\varrho(c)\,\mathrm{d}c$-mixture of the processes $Q_t^{II,c}$

3 Survey of earlier results

In this section we summarize the previous results – rigorously proved and numerical – regarding various limits for the motion of the tagged particle in the model of type I. In Section 4 we formulate and prove a new result concerning the $M \to 0$ asymptotic behaviour of these systems. In Section 5 we describe our new numerical results for the Type II model. These, in view of the result from Section 4, provide information on the $M \to 0$ behaviour of the Type I dynamics as well.

In all cases we are interested in the *diffusive scaling limit of the displacement of the tagged particle motion*, that is in the asymptotics of the rescaled process

$$t \mapsto A^{-1/2} Q_{At}, \quad \text{as} \quad A \to \infty.$$

Throughout the paper we denote this scaling parameter by A .

We briefly survey the existing results on the asymptotics of the tagged particle motion in the model of type I in historical order. The constants

$$\underline{\sigma}^2 := \sqrt{\pi/8} \approx 0.627\ldots, \qquad \overline{\sigma}^2 := \sqrt{2/\pi} \approx 0.798\ldots$$

will play a key role in the formulation of these results.

3.1 The $M = 1$ case:

The case when the tagged particle has the same mass as the rest of the gas particles was investigated and solved in Spitzer (1969) [19]. For the roots of these ideas see also Harris (1965) [8]. In [19] the following invariance principle is proved:

$$\text{for } M = 1: \qquad A^{-1/2} Q_{At}^{I,M} \Rightarrow \overline{\sigma} W_t, \quad \text{as} \quad A \to \infty,$$

where $\Rightarrow$ stands for weak convergence of the sequence of *processes* (see [2] for weak convergence of processes), and W_t is a standard 1-d Brownian motion. That is: $\overline{\sigma} W_t$ is a Brownian motion of variance $\overline{\sigma}^2$.

3.2 The Ornstein-Uhlenbeck limit:

Holley (1971) [9] considers the limit when the mass of the tagged particle is rescaled in the same order as the time scale factor. That is, let $m \in (0, \infty)$ be fixed. Then

$$\text{for } M = mA: \qquad \big(A^{1/2} V^{I,M}_{At}, A^{-1/2} Q^{I,M}_{At}\big) \Rightarrow \big(\eta^m_t, \xi^m_t\big), \qquad \text{as} \qquad A \to \infty,$$

where η^m_t and ξ^m_t are the Ornstein-Uhlenbeck velocity, respectively, position processes defined by the SDEs

$$\mathrm{d}\eta^m_t = -\gamma(m)\eta^m_t\,\mathrm{d}t + \sqrt{D(m)}\,\mathrm{d}W_t, \quad \xi^m_t = \int_0^t \eta^m_s ds,$$

with friction and dispersion parameters

$$\gamma(m) := \frac{4}{m}\sqrt{\frac{2}{\pi}}, \quad D(m) := \frac{8}{m^2}\sqrt{\frac{2}{\pi}}.$$

For a version in higher dimensions of this type of result see Dürr, Goldstein, Lebowitz (1981) [6].

It is important to remark (see [22]), that

$$\xi^m_t \Rightarrow \underline{\sigma} W_t, \qquad \text{as} \qquad m \to 0.$$

This means that taking first Holley's limit, then $m \to 0$ we obtain a Wiener process of variance $\underline{\sigma}^2$ as the diffusive scaling limit of the displacement of the tagged particle.

3.3 Bounds for the limiting variance for any M:

Sinai, Soloveichik (1986) [16] and Szász, Tóth (1986) [21], respectively, consider the case of arbitrary fixed mass M of the tagged particle. In these papers very similar results are proved in completely different ways. These results can be summarized as follows:

$$\text{for } M \ll A: \qquad \underline{\sigma}^2 t \le \liminf_{A\to\infty} \mathbf{Var}\big(A^{-1/2} Q^{I,M}_{At}\big) \le \limsup_{A\to\infty} \mathbf{Var}\big(A^{-1/2} Q^{I,M}_{At}\big) \le \overline{\sigma}^2 t.$$

Note that these bounds are *independent of the mass of the tagged particle.* For surveys of these results see also [14], [17], [18], [23].

Any rigorous result regarding the mass dependence of the limiting variance

$$\sigma^2_M := \lim_{t\to\infty} \mathbf{Var}\big(t^{-1/2} Q^{I,M}_t\big)$$

remains one of the most interesting open questions in this context till today. The only known case is Spitzer's result $\sigma_1 = \overline{\sigma}$. For numerical results see subsection 3.5 below.

3.4 Large mass Wiener limit:

In order to interpolate between the $M =$ const. cases (see subsection 3.3) and Holley's limit (see subsection 3.2) Szász and Tóth (1987) [22] considered the limit with asymptotics $1 \ll M \ll A$, as $A \to \infty$. Here the main result is the following invariance principle:

$$\text{for } A^{1/2+\varepsilon} \ll M \ll A : \qquad A^{-1/2} Q^{I,M}_{At} \Rightarrow \underline{\sigma} W_t, \quad \text{as} \quad A \to \infty. \tag{7}$$

Actually, the scaling limit (7) should hold for $1 \ll M \ll A$ but the method of proof in [22] based on a coupling argument breaks down for $1 \ll M \ll A^{1/2+\varepsilon}$. For a survey of the results recalled in this and the previous paragraph see also [23].

3.5 Earlier numerical results

Following [16] and [21], various numerical investigations were performed in order to establish the mass dependence of the limiting variance: $M \mapsto \sigma^2_M$.

The relevant numerical investigations performed in the late eighties and early nineties are published in Omerti, Ronchetti, Dürr (1986) [12], Khazin (1987) [10], Boldrighini, Cosimi, Frigio (1990) [3], Fernandez, Marro (1993) [7]. These results clearly suggest the qualitative dependence $M \mapsto \sigma^2_M$ shown in Figure 2.

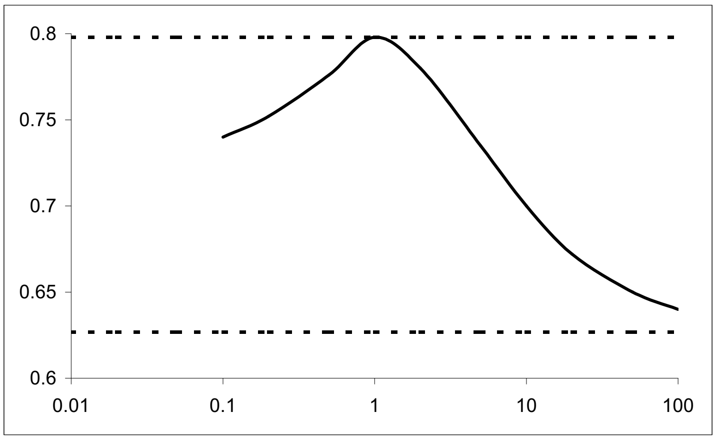

Figure 2: Qualitative dependence $M \mapsto \sigma^2_M$ suggested by earlier numerical works

Regarding the $M \to 0$ limit: in all these papers it is remarked that the numerical simulations for small mass of the tagged particle are unreliable due to instability. On the other hand there was agreement between all researchers interested in these questions that $\lim_{M\to 0}\sigma_M^2 = \overline{\sigma}^2 \approx 0.798\ldots$ should hold. The "straightforward argument" was the following: the tagged particle of extremely small mass must have very small effect on the system, vanishing as $M \to 0$. So, in the $M \to 0$ limit the displacement of any marked particle (in particular the one next to the right of the tagged particle) will asymptotically behave exactly like the tagged particle in Spitzer's equal mass case, cf. subsection 3.1 above. So, the more recent and more accurate numerical results published in Boldrighini, Frigio, Tognetti (2002) [4], suggesting that

$$\lim_{M\to 0}\sigma_M^2 =: \sigma_0^2 \approx 0.74\ldots \tag{8}$$

which is *strictly* inbetween $\underline{\sigma}^2 \approx 0.627\ldots$ and $\overline{\sigma}^2 \approx 0.798\ldots$, *came as a surprise.*

The results of the present note provide substantial theoretical and independent numerical support of this surprising fact.

4 The $M \to 0$ limit of dynamics of type I

Theorem 1. *Let $z \in \mathbb{R}^+$, $u \in [-1,1]$, $W \in \mathbb{R}$ be fixed, $M_n \to 0$, $V_n = M_n^{-1/2}W_n$ so that $W_n \to W \in \mathbb{R}$, and define $c := |Wz|$. Choose $\omega^\pm \in \Omega^\pm$ so that for all n the dynamical trajectories $\mathcal{S}_t^{I,M_n}(\omega^+,\omega^-,z,u,V_n)$ and $\mathcal{S}_t^{II,c}(\omega^+,\omega^-,z)$ are well defined for all $t \in [0,\infty)$. (Note that for any choice of z, u, W and sequences M_n, V_n these $\omega^\pm$-s are of full $\mu^\pm$ measure in $\Omega^\pm$.) Then for all $t \in [0,\infty)$*

$$\lim_{n\to\infty}\Pi\mathcal{S}_t^{I,M_n}(\omega^+,\omega^-,z,u,V_n) = \mathcal{S}_t^{II,c}(\omega^+,\omega^-,z).$$

The convergence is uniform on compact intervals of time.

Proof. Within this proof it is convenient to describe the systems of particles as seen from a fixed external frame of reference: the position of the tagged particle (in the system of type I) at time t is $Q_t^{I,M}$, the positions of the untagged gas particles are $y_{\pm i}(t)$, $i = 1,2,\ldots$, as given in (5).

We have to prove that in the limit described in the theorem the trajectories of the particles in system I converge to the corresponding trajectories in the limit system of type II. Note that the particles with $i \neq \pm 1, 0$ follow the same dynamical rules in the two types of dynamics. Thus we only need to understand how the motion of the particles with indices ± 1 can be approximated as $M \to 0$, if they interact with the tagged particle according to the rules of section 2.2.1.

Let us investigate the model of the type I for some fixed nonzero $M \ll 1$. In what follows we will consider intervals of time in which collisions neither between the particles of indices -1 and -2, nor between those of indices 1 and 2 occur. Note that for such intervals the three central particles (of index $0, \pm 1$) form an isolated subsystem. How the dynamics are effected by collisions between the particles of indices i and j, where $i = \pm 1$ and $j = \pm 2$, will be discussed at the end of the proof.

As mentioned above, the particles with indices -1, 0 and 1 have positions $y_{-1}(t) \leq Q_t \leq y_1(t)$ and velocities $v_{-1}(t)$, $V_t = W_t/\sqrt{M}$ and $v_1(t)$, respectively, where $v_{\pm 1}(t)$ and W_t are of order one. One more quantity of interest is $z(t) := y_1(t) - y_{-1}(t)$, the distance of the particles with indices ± 1. For brevity we often omit the dependence on t when considering these quantities.

As V is very large, the tagged particle performs a full cycle: it hits one of its neighbours, turns back, collides with the other neighbour, and gets back to its initial position within a very short time $\mathrm{d}t$. See Figure 3 for insight.

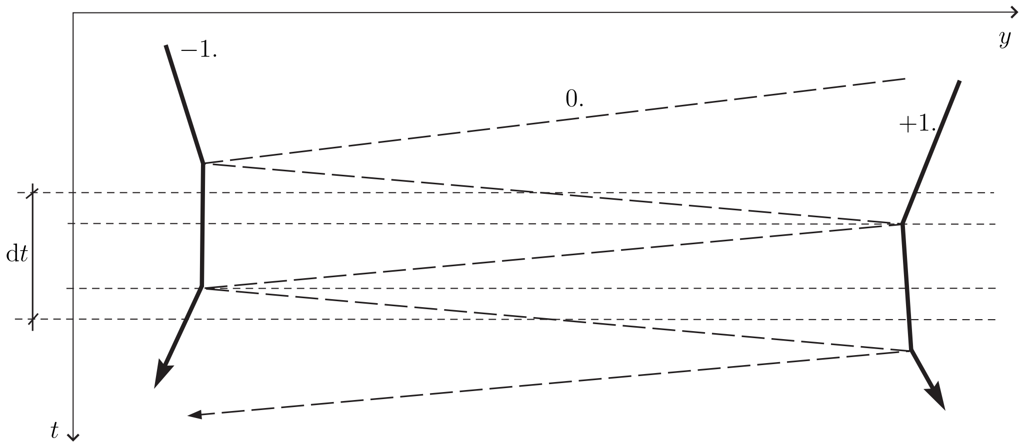

Figure 3: Successive collisions of the tagged particle of mass $M \ll 1$ with its neighbours

We argue as follows. We obtain difference equations that describe how the relevant quantities (W, z, v_1, v_{-1} etc.) evolve during the above mentioned cycles, for an arbitrary fixed, small, however, nonzero M. The time step of these difference equations will be the length of the cycle, that is, $\mathrm{d}t$. Then we will see that as $M \to 0$, $\mathrm{d}t \to 0$ as well, and, furthermore, the difference equations limit to differential equations corresponding to the statement of the Theorem.

To investigate how the system evolves in the time interval $\mathrm{d}t$, two successive collisions should be taken into account. We may assume that $W > 0$ (the case of negative W is analogous), and thus the tagged particle collides first with the particle of index 1, and then with that of index -1. These collisions split the time interval into three smaller subintervals. Let us expand the formulas of (4) in the limit as $M \to 0$. This way we may calculate the velocities of the three particles in the three subintervals, see Table 1. Observe that the order of magnitude of the incoming velocities are as follows:

$$V = W/\sqrt{M} \asymp M^{-1/2}, \qquad v_{\pm 1} \asymp 1.$$

In particular, the tagged particle reverts its velocity at collisions, thus its speed is constant, more precisely, equal to $|V| + \mathcal{O}(1) = |W/\sqrt{M}| + \mathcal{O}(1)$ throughout the investigated

	1. interval	2. interval	3. interval
particle 1	v_1	$v_1 + 2MV + \mathcal{O}(M)$	$v_1 + 2MV + \mathcal{O}(M)$
particle 0	V	$-V + 2v_1 + \mathcal{O}(\sqrt{M})$	$V - 2v_1 + 2v_{-1} + \mathcal{O}(\sqrt{M})$
particle -1	v_{-1}	v_{-1}	$v_{-1} - 2MV + \mathcal{O}(\sqrt{M})$

Table 1: Velocities in the $M \to 0$ approximation

time interval. This implies $dt \asymp \sqrt{M}$. Furthermore, the velocities v_1 and v_{-1} remain $\mathcal{O}(1)$, and thus, the particles of index 1 and -1 remain $\mathcal{O}(\sqrt{M})$-close to their original positions y_1 and y_{-1} in the investigated interval. By the above observations the distance of the two non-tagged particles remains $\mathcal{O}(\sqrt{M})$-close to z. Now we may calculate the leading term in $\mathrm{d}t$:

$$\mathrm{d}t = \frac{2z + \mathcal{O}(\sqrt{M})}{V + \mathcal{O}(1)} = \frac{2z}{W}\sqrt{M} + \mathcal{O}(M). \tag{9}$$

Let us denote the amount with which the velocities change at the collisions (and thus, during the studied time interval $\mathrm{d}t$) by $\mathrm{d}v_1$ and $\mathrm{d}v_{-1}$.

Referring to Table 1 we get

$$\mathrm{d}v_1 = 2W\sqrt{M} + \mathcal{O}(M), \qquad \mathrm{d}v_{-1} = -2W\sqrt{M} + \mathcal{O}(M). \tag{10}$$

Referring again to Table 1, we may calculate the amount of change in the velocity of the tagged particle during the time interval $\mathrm{d}t$. We get

$$\mathrm{d}V = 2v_{-1} - 2v_1 + \mathcal{O}(\sqrt{M}), \qquad \text{thus} \qquad \mathrm{d}W = \sqrt{M}(2v_{-1} - 2v_1) + \mathcal{O}(M). \tag{11}$$

On the basis of (10) and (9) it is also possible to find the leading term in the change of z during the cycle:

$$\mathrm{d}z = (v_1 - v_{-1})\,\mathrm{d}t + \mathcal{O}(M) = \frac{2z}{W}\sqrt{M}(v_1 - v_{-1}) + \mathcal{O}(M). \tag{12}$$

Now (11) and (12) together imply:

$$W\,\mathrm{d}z = -z\,\mathrm{d}W + \mathcal{O}(M)$$

and thus

$$\mathrm{d}(Wz) = \mathcal{O}(M) = o(dt). \tag{13}$$

In what follows we consider the $M \to 0$ limit of the coupled difference equations (9), (10) and (13). On the one hand we find that $|Wz|$ is an integral of motion in the sense that in the $M \to 0$ limit $c = |W(t)z(t)|$ is *constant*. Furthermore, the difference equations (9) and (10) together imply that, as $M \to 0$, $v_1(t)$ and $v_{-1}(t)$ approach (piecewise) differentiable functions, and

$$\dot{v}_1 = \frac{W^2}{z} = \frac{c^2}{z^3}, \qquad \dot{v}_{-1} = -\frac{W^2}{z} = -\frac{c^2}{z^3}. \tag{14}$$

Altogether we find that the positions and velocities for the particles with indices ± 1 satisfy the coupled differential equations

$$\begin{aligned} \dot{x}_1 &= v_1, & \dot{v}_1 &= c^2/z^3, \\ \dot{x}_{-1} &= v_{-1}, & \dot{v}_{-1} &= -c^2/z^3. \end{aligned} \tag{15}$$

This is in agreement with the Formula (6) for the potential that appears in the definition of the type *II* dynamics.

Our argument applies so far to a time interval when the tagged particle has the same neighbours. Notice now that the value of $c = |W(t)z(t)|$ also remains constant when one of the neighbours of the tagged particle 'meets' another gas particle, and the neighbour is replaced by that new particle. At such a time moment the values of both W and z are unchanged. Thus for any $t > 0$ $|W(t)z(t)| = |W(0)z(0)| = c$ according to the choice of c in the formulation of Theorem 1. Thus, after such a collision between the particles of indices 1 and 2 (or between those of indices -1 and -2) the two central particles evolve according to the same system of differential equations – that is, (15) – as before such a collision. However, as the velocity v_1 (or v_{-1}) changes instantaneously, the subsystem of the two central particles jumps to another trajectory of (15). This is in agreement with the dynamics of the model of type II, cf. the description in Section 2.2.2. Thus the proof of Theorem 1 is complete. □

Remark. *It is worth noting that – with analogous arguments – one could first obtain differential equations that – in the limit as $M \to 0$ – describe the evolution of the quantities W and z, and conclude thereafter that $c = |Wz|$ is an integral of motion.*

Remark. Note that taking the $c \to 0$ limit of the dynamics of type *II*, we recover the dynamics of type *I* with equal masses: the interaction between the two central particles becomes hard core specular collision. So, in this double limit ($M \to 0$ and then $c \to 0$) the system indeed behaves as Spitzer's model, see subsection 3.1.

Recall that according to (3) the measure μ^{II} which is the projection of the measures $\mu^{I,M}$ on the state space Ω^{II}, is the $\varrho(c)\,\mathrm{d}c$-mixture of the Gibbs measures $\mu^{II,c}$. This implies that Theorem 1 has the following immediate corollary:

Corollary. *Let $M \to 0$. For any fixed $0 < T < \infty$, the sequence of processes $[0,T] \ni t \mapsto \widetilde{Q}_t^{I,M}$ converges weakly (in distribution) to the process $[0,T] \ni t \mapsto Q_t^{II}$.*

5 Numerical results on systems of type II

5.1 Generalities

In this section we describe numerical investigations aimed at calculating the limiting variance

$$\sigma^2 := \lim_{t\to\infty} t^{-1}\mathbf{Var}\big(Q_t\big)$$

for the systems of type II. We shall also comment on how these results are related to the $M \to 0$ limit of the variance for the systems of type I, as established numerically in [4].

These simulations of the systems of type II were done by following a number of particles for some fixed time T. The particles followed were those who were less than $10T$ far away from the point of observation in the beginning. It is easy to check that with this method the probability of not following a particle that would indeed participate in the interaction is negligible in all the cases we looked at.

Numerical simulation of the dynamics of type II is relatively fast, since the equation of motion for the two particles interacting via the potential (6) can be solved explicitly. (This observation is at the heart of the complete solvability of the Calogero-Moser-Sutherland model.)

The simulation for time T was repeated over a sample of N initial conditions chosen independently according to the appropriate stationary Gibbs distribution. From this sample, the empirical variance was calculated for $\mathbf{Var}\big(Q_t\big)$ as a function of t.

The result of a typical simulation can be seen in Figure 4. The solid line is the best linear fit for the tail, while the dashed lines have slope $\underline{\sigma}^2$ and $\overline{\sigma}^2$, and are drawn for comparison.

As we can see, $\mathbf{Var}\big(Q_t\big)$ does appear to be asymptotically linear. To read the limit $\lim\limits_{t\to\infty} t^{-1}\mathbf{Var}\big(Q_t\big)$ from the graph, we needn't perform a simulation so long that this limit is well approached: the slope of the asymptote can be found with good accuracy much sooner. Thus all the limits given in the paper are obtained using this technique, and the time interval for the simulation is typically between $T = 10$ and $T = 50$. In exchange, the size of the sample can be very big – actually, samples up to $N = 10^7$ were used.

Finally, the statistical error of the calculated values was estimated by simply repeating the whole procedure about 20 times and calculating the standard deviation of the values obtained.

A detailed description of the numerical simulation and the source code for the applied program can be found in [25].

5.2 The systems with fixed c

We simulated numerically the dynamics of type II for various fixed values of the parameter c ranging between 0.01 and 100. We started the system from samples of the

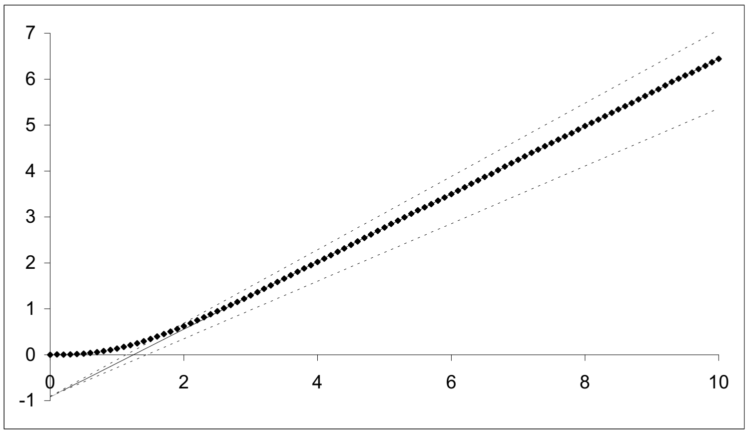

Figure 4: $\mathbf{Var}\big(Q_t\big)$ as a function of t in a typical simulation

stationary Gibbs distribution $\mu^{II,c}$ and computed the limiting variance

$$\sigma_c^2 := \lim_{t\to\infty} t^{-1}\mathbf{Var}\big(Q_t^{II,c}\big).$$

We found the $c \mapsto \sigma_c^2$ dependence of the limiting variance as shown in Figure 5. We see that $\lim_{c\to 0}\sigma_c^2 \to \overline{\sigma}^2$, which is no surprise, since in the $c \to 0$ limit the system indeed behaves like the system of type I with $M = 1$, which is known to have $\sigma_{M=1}^2 = \overline{\sigma}^2$. See subsection 3.1 and the Remark after the proof of Theorem 1.

On the other hand, it is interesting to see that as $c \to \infty$, the limiting variance decreases, and even seems to approach a value near the lower limit $\underline{\sigma}^2$, but not quite reaching this lower bound. We plan to return to this phenomenon in the forthcoming paper [1].

5.3 The mixed system

We computed the numerical value of the limiting variance for the mixture dynamics in two different ways.

First, we computed numerically the value of

$$\sigma_{\mathrm{mix},1}^2 := \lim_{t\to\infty} t^{-1}\mathbf{Var}\big(Q_t^{II}\big).$$

We did it in the following way: we sampled the initial conditions ω^{II} according to the distribution μ^{II} and, independently, a standard normal variable W. Then we computed

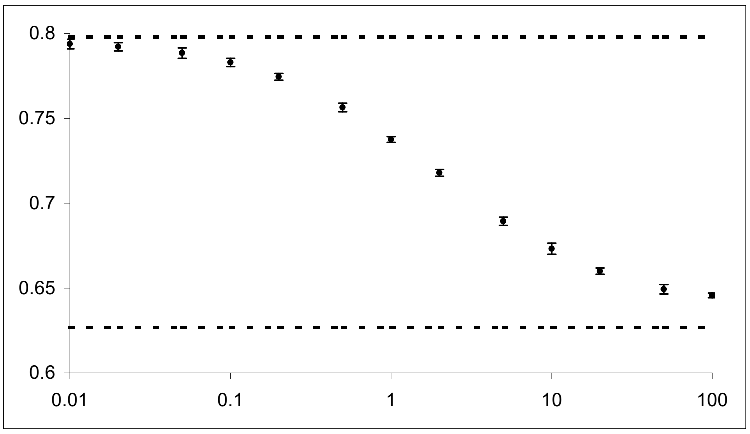

Figure 5: c-dependence of the limiting variance for systems of type II

$c := |Wz|$, where z was the distance between the two central particles in the initial configuration ω^{II}. This *random* value c served as the strength parameter in the interaction potential (6), with which the dynamics $\mathcal{S}_t^{II,c}$ were computed.

Second, using the data obtained for σ_c^2 in the fixed c computations (see subsection 5.2), we computed the mixture

$$\sigma^2_{\mathrm{mix},2} := \int_0^\infty \sigma_c^2 \rho(c)\,\mathrm{d}c,$$

which, of course, in principle must give the same value as the previous computation.

Indeed, in the two cases we obtained the numerical values

$$\sigma^2_{\mathrm{mix},1} = 0.736 \pm 0.003, \quad \sigma^2_{\mathrm{mix},2} = 0.740 \pm 0.003.$$

This result is very interesting, since it coincides exactly (well within statistical error) with the $M \to 0$ limit of the variance calculated numerically in [4], see (8). This means that there is indeed *continuity* in the limiting variance as $M \to 0$.

We remark that the function $c \mapsto \sigma_c^2$ shown in Figure 5 can be fit with amazing accuracy by the function of the simple form $\sigma_c^2 = \frac{A_1 - A_2}{1+\left(\frac{c}{c_0}\right)^p} + A_2$, where $A_1 = 0.796$, $A_2 = 0.638$, $c_0 = 1.981$, $p = 0.792$.

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