4.4: Long-time Tails and Mode-coupling Theory

The Problem

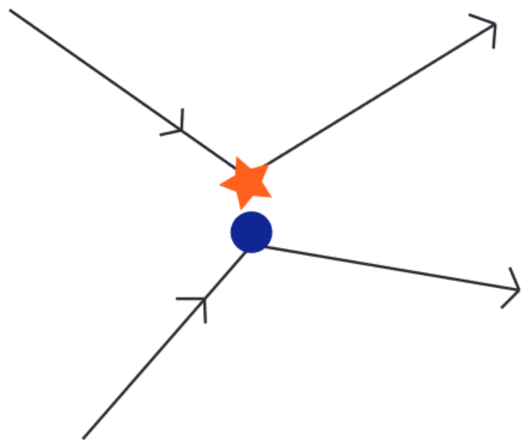

Figure 4.4: Uncorrelated collision of two particles in a fluid

where the memory kernel is related to the diffusion constant through Einstein's relation

[Math Processing Error]

In 1967, Alder and Wainwright used computer simulations to calculate the velocity correlation function of hard-sphere gases [6]. They found that at long times, *[Math Processing Error]* exhibits a power-law decay rather than an exponential decay. That is, *[Math Processing Error]* decays according to *[Math Processing Error]*

[Math Processing Error]

This is the famous long-time tail problem in kinetic theory.

Memory Effects

The fundamental assumption underlying the exponential decay model of the velocity correlation function is that collisions between particles in a dilute hard-sphere gas are independent. This means that after each collision, a particle will lose memory of its original velocity until its motion has become completely randomized. This assumption leads to the exponential decay *[Math Processing Error]*, where *[Math Processing Error]* is the average collision time.

However, it is also possible that collisions are not completely independent but instead are correlated. A correlation would occur if, for example, two particles collide and then collide again after undergoing some number of other collisions (see Figures *[Math Processing Error]* and 4.6). This implies that there is a long term memory in the system which would lead to a decay that is slower than an exponential.

To estimate the form of this decay, we can consider the probability that, following a collision, a particle remains at or returns to its initial position after a time t, *[Math Processing Error]*. To make a rough estimate of this probability, imagine that at any moment in time we can draw a "probability sphere" for the particle. The probability of finding the particle inside the sphere is constant, and the probability of finding the particle outside the sphere is zero. At time *[Math Processing Error]*, the particle has not had time to travel away from its initial position. Therefore, *[Math Processing Error]*. As *[Math Processing Error]* increases, the particle begins to diffuse away from its initial position. The radius of the sphere increases linearly

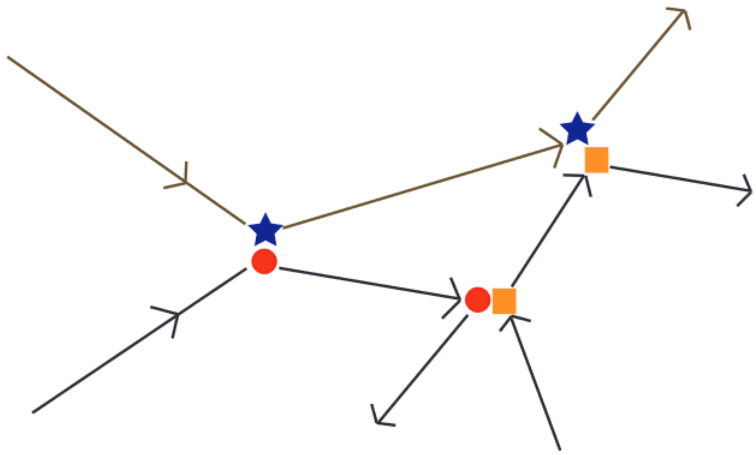

Figure 4.5: A test particle (blue star) collides with one particle (red circle), altering that particle’s trajectory such that it collides with a third particle (yellow square). The subsequent collision of the third particle with the test particle is correlated with the initial collision.

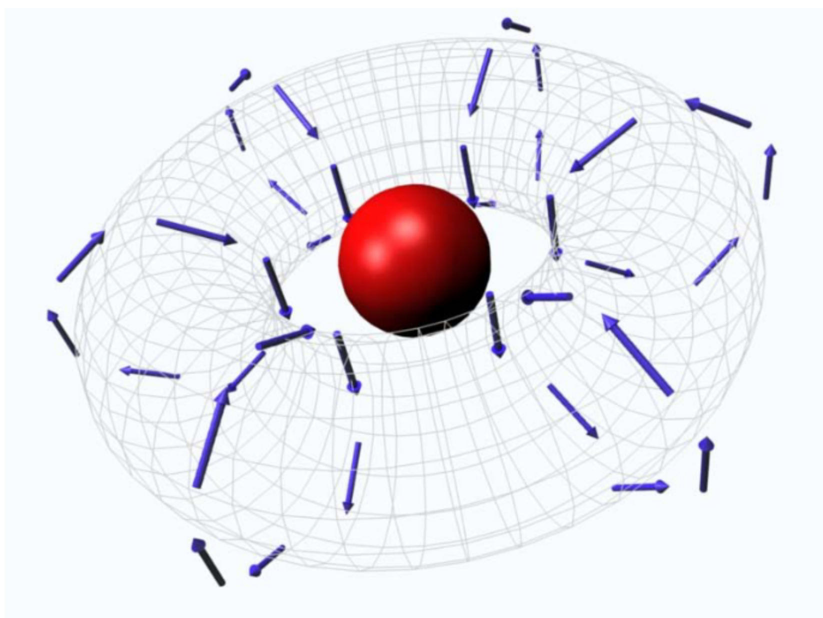

Figure 4.6: Vortex rings in the fluid around a hard sphere particle can contribute to the long-time tail of the velocity autocorrelation function [6]. with time according to *[Math Processing Error]*, where *[Math Processing Error]* is the diffusion constant.

To estimate *[Math Processing Error]* from probability sphere, note that the probability of finding the particle at any point in space must be unity:

[Math Processing Error]

We only need to integrate over the volume of the sphere, since the probability of finding the particle anywhere else is zero. Within the sphere, the probability is a constant, *[Math Processing Error]*. Therefore, this integral simplifies to

[Math Processing Error]

The volume of the sphere goes as *[Math Processing Error]*, where *[Math Processing Error]* is the spatial dimension. Therefore, the probability goes as

[Math Processing Error]

For a three dimensional system, we get a result consistent with Alder and Wainwright’s predictions

[Math Processing Error]

This shows that memory effects may be the source of the power law decay.

We can construct a simple model of the behavior of a system for which memory effects are important. In this model, a particle with a velocity *[Math Processing Error]* creates a velocity field through its interactions with other particles. This velocity field can in turn influence the long time behavior of the particle.

We can start by getting a rough estimate of this velocity field from the transverse current

[Math Processing Error]

where *[Math Processing Error]* is the diffusion constant, *[Math Processing Error]* is the shear viscosity, and *[Math Processing Error]*. The transverse current is written in *[Math Processing Error]*-space. By transforming this into real space, we obtain an expression for the dissipation of the velocity field over time and space

[Math Processing Error]

The velocity field dissipates due to friction. At short times, the decay has a Gaussian form. However, at long times the decay is dominated by the prefactor, which goes as *[Math Processing Error]*.

Hydrodynamic Model

A simple way of deriving the above result would be to evaluate the velocity correlation function

[Math Processing Error]

Using the hydrodynamic model, we can find this correlation function by taking the equilibrium average of the non-equilibrium average thermal velocity

[Math Processing Error]

where *[Math Processing Error]* is the Boltzmann distribution and *[Math Processing Error]* is a non-equilibrium velocity field:

[Math Processing Error]

Here, *[Math Processing Error]* describes the tagged particle.

The non-equilibrium velocity field can be represented as a coupling of the linear modes *[Math Processing Error]* and *[Math Processing Error]*

[Math Processing Error]

We can solve this using the solutions of the hydrodynamic modes:

[Math Processing Error]

For transverse modes,

[Math Processing Error]

Then, take the equilibrium average

[Math Processing Error]

Finally,

[Math Processing Error]

Mode-Coupling Theory

As shown above, the correlation of a given dynamic quantity decays predominantly into pairs of hydrodynamic modes with conserved variables. Mode-Coupling Theory is the formalism that calculates their coupling.

From the discussion about, the velocity of the tagged particle is coupled to a bilinear mode, *[Math Processing Error]*. then

[Math Processing Error]

where *[Math Processing Error]* is the projection operator associated with *[Math Processing Error]*. By expanding the projection operator

[Math Processing Error]

Now, use the linear hydrodynamic modes to evaluate the correlation function.

[Math Processing Error]

Then

[Math Processing Error]

and

[Math Processing Error]

so that

[Math Processing Error]

Therefore,

[Math Processing Error]

Now,

[Math Processing Error]

and

[Math Processing Error]

Then

[Math Processing Error]

By incorporating the three-spatial components of [Math Processing Error] and [Math Processing Error], we have

[Math Processing Error]

References

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