Tagged particle diffusion in single-file systems

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J. Stat. Phys. **160**, 73 (2015),
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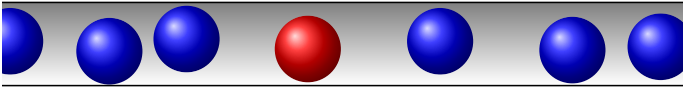
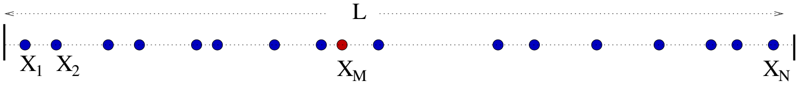
Outline



- Introduction: Tagged particle motion in one dimensional systems
- Hamiltonian systems: effect of integrability
  - Harmonic crystal $\rightarrow$ Fermi-Pasta-Ulam chain
  - Equal mass hard point gas $\rightarrow$ Alternate mass hard point gas
- General approach for “identity-exchange” dynamics:-
  Large deviations and two-particle distributions.
- Conclusions



Let $\Delta x(t) = x_M(t) - x_M(0)$.
Consider the correlation functions $\langle [\Delta x(t)]^2 \rangle$, $\langle \Delta x(t) v(0) \rangle$ and $\langle v(t) v(0) \rangle$.

$$D(t) = \frac{1}{2} \frac{d}{dt} \langle [\Delta x(t)]^2 \rangle = \int_0^t \langle v(0) v(t') \rangle dt' = \langle \Delta x(t) v(0) \rangle \ .$$

The average is over thermal initial conditions (and also over trajectories, for stochastic dynamics).

Let $N/L = \rho$.
If $D = \lim_{t \to \infty} \lim_{L \to \infty} D(t)$ is finite, then we say tagged particle motion is diffusive,

$$\text{thus} \quad \langle [\Delta x(t)]^2 \rangle = 2Dt \ .$$

$D \to 0$ implies sub-diffusion and $D \to \infty$ implies super-diffusion.

Review of earlier work

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 6, NUMBER 3 MARCH 1965

Dynamics of a Simple Many-Body System of Hard Rods

D. W. Jepsen
IBM Watson Research Center, Yorktown Heights, New York
(Received 17 July 1964)

General formulas are given for the exact calculation of the nonequilibrium properties of the one-dimensional system of equal-mass hard rods both for a finite but large system and in the limit of infinite size. Only properties which depend upon labeling one or more of the particles are nontrivial in this system. Various results are obtained on Poincaré cycles, delocalization of a particle with time and electrical conductivity when one particle is charged.

- One dimensional gas with Hamiltonian dynamics – equal mass particles moving balistically between elastic collisions.
- Exact results for infinite system with a fixed density n of particles —

$$\langle [x(t) - x(0)]^2 \rangle \sim 2Dt \,, \qquad D = \frac{1}{n}\sqrt{\frac{k_B T}{2\pi m}} \,,$$

$$\langle v(t) v(0) \rangle \sim \sqrt{\frac{m}{2\pi k_B T}}\left(-1 + \frac{5}{2\pi}\right)\frac{1}{n^3 t^3} \,.$$

Averaging is over thermal initial conditions.

Review of earlier work

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 1, NUMBER 1 JANUARY–FEBRUARY, 1960

Poincaré Cycles, Ergodicity, and Irreversibility in Assemblies of Coupled Harmonic Oscillators*

PETER MAZUR
Institute Lorentz, Leiden, The Netherlands

AND

ELLIOTT MONTROLL
Institute for Fluid Dynamics and Applied Mathematics, University of Maryland, College Park, Maryland

(Received January 10, 1960)

The transport coefficients (diffusion constant, electrical conductivity, etc.) associated with irreversible processes in an assembly of particles can be expressed as integrals over certain time relaxed correlation functions between small numbers of variables of the assembly. The scattering of slow neutrons is also a measure of time relaxed correlation functions.

Irreversibility is a consequence of the vanishing of the correlation coefficients as the relaxation time becomes infinite. On the other hand these coefficients have Poincaré cycles so that any value which they take on is repeated an infinite number of times. It is shown that, in the case of fluctuations of $0(N^{-\frac{1}{2}})$ from zero (N being the number of degrees of freedom), the period of Poincaré cycles is of the order of the mean period of normal mode vibrations while for fluctuations of a magnitude independent of N the period is of the order of C^N where C is a constant which is greater than 1.

The time relaxed correlation coefficients of a pair of particles separated by r lattice spacings decays as $t^{-m/2}$, m being the number of dimensions of the assembly. The statistics of the decay of the momentum of a particle from a preassigned initial value to its equipartition value are discussed.

- Harmonic crystals — Exact results for infinite systems—

Finite diffusion constant

$$D = \frac{k_B T}{2\rho c} \qquad \rho = m/a, \quad c = a\sqrt{k/m}$$

$$\langle v(t)v(0)\rangle \sim \frac{sin(\omega_0 t)}{(2\pi\omega_0 t)^{1/2}} .$$

Averaging is over thermal initial conditions.

J. Appl. Prob. 2, 323-338 (1965)
Printed in Israel

DIFFUSION WITH "COLLISIONS" BETWEEN PARTICLES

T. E. HARRIS, *The Rand Corporation*
(*University of Southern California from February* 1966)

- One dimensional gas with Brownian dynamics – particles freely diffusing but with no-crossing condition. Similar to simple exclusion process.
- Exact results for infinite system with a fixed density $n = N/L$ of particles —

$$\langle [x(t) - x(0)]^2 \rangle \sim \frac{2}{n}\sqrt{\frac{Dt}{\pi}} \, .$$

Averaging is over thermal initial conditions and also stochastic paths.

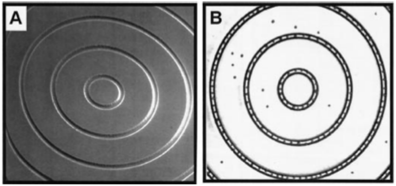
Thus the caging effect of single file diffusion leads to a subdiffusive motion of particles.

Science **287**, 5453 (2000).

Single-File Diffusion of Colloids in One-Dimensional Channels

Q.-H. Wei,*† C. Bechinger,* P. Leiderer

Single-file diffusion, prevalent in many processes, refers to the restricted motion of interacting particles in narrow micropores with the mutual passage excluded. A single-filing system was developed by confining colloidal spheres in one-dimensional circular channels of micrometer scale. Optical video microscopy study shows evidence that the particle self-diffusion is non-Fickian for long periods of time. In particular, the distribution of particle displacement is a Gaussian function.



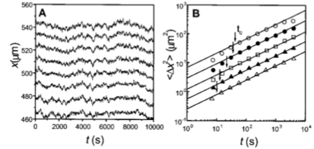


Fig. 2. (**A**) Typical trajectories for eight neighboring particles in the largest channel in Fig. 1A. The instantaneous particle coordinates were extracted from digitized pictures with an image-processing algorithm and saved in a computer for later analysis. From those data, we obtained the particle trajectories. The system was equilibrated for at least 4 hours before each measurement. To obtain the long-time behavior, we recorded the coordinates of colloidal particles for ~8 hours, with a time interval of ~8 s between two adjacent pictures. (**B**) Log-log plot of the measured particle MSDs versus the observation time for five different particle interaction strengths Γ: 0.66, open circles; 1.1, solid circles; 2.34, open squares; 4.03, solid triangles; and 7.42, open triangles. The data points have been shifted upward by ln 2 for clarity, and the solid lines are best fit with Eq. 1 with the mobility F as an adjustable parameter.

Experiments

PRL **94,** 216001 (2005) PHYSICAL REVIEW LETTERS week ending 3 JUNE 2005

From Random Walk to Single-File Diffusion

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Haim Diamant
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(Received 5 January 2005; published 2 June 2005)

We report an experimental study of diffusion in a quasi-one-dimensional (q1D) colloid suspension which behaves like a Tonks gas. The mean squared displacement as a function of time is described well with an ansatz encompassing a time regime that is both shorter and longer than the mean time between collisions. The ansatz asserts that the inverse mean squared displacement is the sum of the inverse mean squared displacement for short time normal diffusion (random walk) and the inverse mean squared displacement for asymptotic single-file diffusion (SFD). The dependence of the 1D mobility in the SFD on the concentration of the colloids agrees quantitatively with that derived for a hard rod model, which confirms for the first time the validity of the hard rod SFD theory. We also show that a recent SFD theory by Kollmann [Phys. Rev. Lett. **90**, 180602 (2003)] leads to the hard rod SFD theory for a Tonks gas.

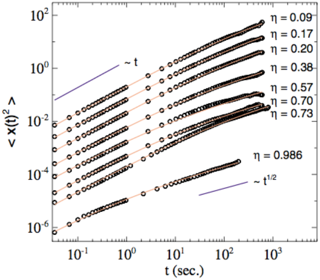


FIG. 2 (color online). Mean squared displacement as a function of t at different concentrations. Note that $\langle x(t)^2\rangle$ for large spheres is scaled by the factor σ_2/σ_1. The data (symbols) are shifted downward a factor of 3 from one another for clarity. The error bars are smaller than the symbols used. For $t \leq 1$ s the movies were grabbed at 30 frames/s, and for $t > 1$ s the images were grabbed at 4 and 5 frames/s for small and large spheres, respectively (only a subset of the data are plotted for clarity). The solid lines are fits of the data to Eq. (8).

Some open questions

- The equal mass HP gas and the harmonic chain are both very special systems — both are integrable models. What happens with more realistic models ? Do we still get diffusion in systems with any generic Hamiltonian dynamics ?
  Relation to thermal conduction studies ?
- Finite size effects. Eventually, in any finite system, the mean square displacement will stop growing with time and will saturate to a finite value determined by the equilibrium distribution $((\Delta x)^2 \sim N)$. How does this approach to the saturation value take place ?
- If the motion is diffusive, how do we determine the diffusion constant ?
  Prediction from hydrodynamic theory ?
- Mostly the second moment (MSD) has been computed. What about large deviations?

Earlier work – Hamiltonian systems

- Non-integrable dynamics
  Alternate mass HP gas – Marro and Masoliver: Phys. Rev. Lett. 54, 731 (1985)

  $$\langle v(0)v(t)\rangle \sim -\frac{1}{t^{\delta}} \qquad \delta < 1 \ .$$

  This implies a negative divergent diffusion constant and is impossible!

  Lennard Jones gas – Bishop, Derosa and Lalli: J. Stat. Phys. 25, 229 (1981)
  Srinivas and Bagchi: J. Chem. Phys. 112, 7557 (2000).
  Finite diffusion constant and

  $$\langle v(0)v(t)\rangle \sim \frac{1}{t^{3}} \qquad \delta < 1 \ .$$

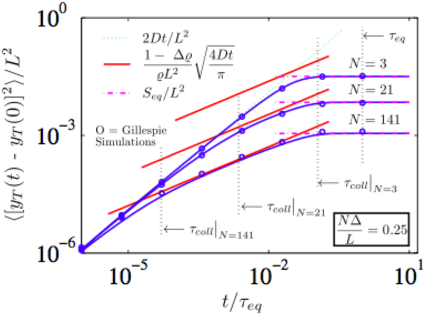
- Finite size effects in equal mass HP gas.
  Some general results have been obtained in —

  Lebowitz and Percus: Phys. Rev. 155, 122 (1967)
  Lebowitz and Sykes: J. Stat. Phys. 6, 157 (1972)
  Percus: J. Stat. Phys. 138, 40 (2010)

  However, the results are mostly formal, and not very explicit.

- Stochastic dynamics — A number of work have studied finite size effects e.g:

  Gupta, Majumdar, Godreche and Barma, Phys. Rev. E 76, 021112 (2007)
  Lizana and Ambjornsson, Phys. Rev. Lett 100, 200601 (2008)
  Barkai and Silbey, Phys. Rev. Lett. 102, 050602 (2009)



Present work — Mostly Hamiltonian systems.

- Finite size effects in harmonic chain and equal mass HP gas — both integrable models.
- Simulation results for FPU chain, alternate mass HP gas and Lennard-Jones gas.
- Analytic results from linearized hydrodynamic theory.
- Hard particle gas and non-crossing Brownian particles: Exact results from mapping to non-intercting particles— Universal large deviation function, two particle correlations.

Time regimes

- "Short time regime" — times at which the tagged particle does not know that the system is finite.
- "Long time regime" — times after which finite size effects start showing up. We use hard walls so that the mean square diplacement eventually saturates.

Harmonic chain

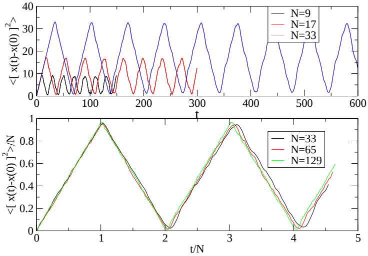
The Hamiltonian of the system is

$$H = \sum_{l=1}^{N} \frac{m}{2} \dot{x}_l^2 + \sum_{l=1}^{N+1} \frac{k}{2} (x_l - x_{l-1})^2 \; .$$

Normal mode frequencies: $\omega_s^2 = (2k/m)\,[1 - \cos(s\pi/(N+1))]$.
A simple analysis, using normal modes gives:

$$\langle [\Delta x(t)]^2 \rangle \;=\; 2\left[\langle x^2(0)\rangle - \langle x(t)x(0)\rangle\right] = \frac{8k_BT}{m(N+1)} \sum_{s=1,3,\ldots} \frac{\sin^2(\omega_s t/2)}{\omega_s^2} \; ,$$

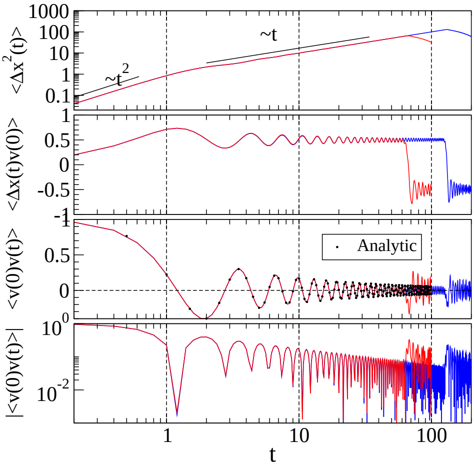
$$\langle v(t)v(0)\rangle \;=\; \frac{2k_BT}{m(N+1)} \sum_{s=1,3,\ldots} \cos(\omega_s t) \; .$$



Long time form of MSD of central particle for small systems, computed from above equations numerically. Frequency and amplitude of oscillations scale with system size.

Note: Short time ($t \lesssim N$) is diffusive.

Harmonic Chain — Short time behaviour



Harmonic chain — Main results

There are three distinct time regimes:

1. When $\omega_N t << 1$, $\sin^2(\omega_n t/2) \approx \omega_n^2 t^2/4$, the MSD is then equal to $k_B T t^2/m$.

2. In the second part, $t >> 1$ and $t/N << 1$ we get

$$\langle [\Delta x(t)]^2 \rangle = \frac{8k_B T}{m(N+1)} \sum_{s=1,3,\dots} \frac{\sin^2(\omega_s t/2)}{\omega_s^2} = \frac{2k_B\, T\, a\, t}{\pi\, m\, c} \int_0^\infty dy \frac{\sin^2(y)}{y^2} = 2D\, t\,,$$

   with the diffusion constant $D = k_B T/(2\rho c)$.

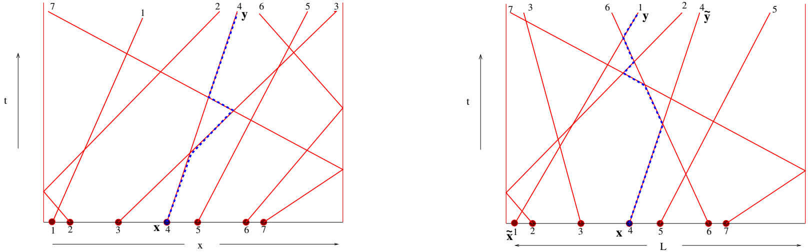
3. "Large times" — there is an almost-periodic behaviour, with the peaks of $\langle (\Delta x)^2 \rangle$ being proportional to N while the minimas almost touch zero. We see that plotting $\langle (\Delta x)^2 \rangle / N$ against t/N gives a good scaling of the data. The near-recurrences ($\sim N^{1/3}$) are somewhat surprising since we are averaging over an initial equilibrium ensemble.
   (Analytic understanding from more careful analysis of sum)

Equal mass hard particle gas

- Gas of $N = 2M + 1$ point particles in a one-dimensional box of length L.
- Particles interact with each other through hard collisions conserving energy and momentum — colliding particles simply exchange velocities.
  When an end particle collides with the adjacent wall, its velocity is reversed.
- Initial state of the system is drawn from the canonical ensemble at temperature T.
  Thus, initial positions of the particles are uniformly distributed in the box.
  Initial velocities of each particle choosen independently from Gaussian distribution with zero mean and a variance $\overline{v}^2 = k_B T/m$.

  Note: Particles are ordered $0 < x_1 < x_2 < \cdots < x_{N-1} < x_N < L$ at all times.

Equal mass hard particle gas – Mapping to non-interacting problem



- One can effectively treat the system as non-interacting — keep track of labels.
- To find the VAF of the middle particle in the interacting-system from the dynamics of the non-interacting system, we note that there are two possibilities in the non-interacting picture

  1. the same particle is the middle particle at both times $t = 0$ and t, or
  2. two different particles are at the middle position at times $t = 0$ and t respectively.

- Denote the VAF corresponding to these two cases by $\langle v_M(0)v_M(t)\rangle_1$ and $\langle v_M(0)v_M(t)\rangle_2$. The complete VAF is given by $\langle v_M(0)v_M(t)\rangle = \langle v_M(0)v_M(t)\rangle_1 + \langle v_M(0)v_M(t)\rangle_2$.

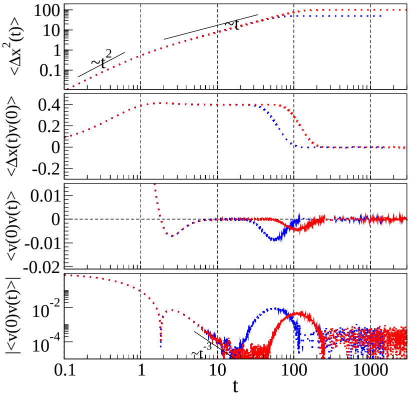
Equal mass hard particle gas – Mapping to non-interacting problem

- To compute $\langle v_M(0)v_M(t)\rangle_1$, —
  (i) Pick one of the non-interacting particles at random,
  (ii) Find the probability that it goes from $(x,0)$ to (y,t),
  (iii) Find probability that it is the middle particle at both $t=0$ and t,
  (iv) Multiplying by $v(0)v(t)$ and integrating over x and y.

- To compute $\langle v_M(0)v_M(t)\rangle_2$, —
  (i) Pick two particles at random at time $t=0$,,
  (ii) Find probability that they go from $(x,0)$ to $(\tilde{y},t)$ and $(\tilde{x},0)$ to $y,t)$,
  (iii) Find probability that there are an equal number of particles on both sides of x and y at $t=0$ and t respectively,
  (iv) Multiply by $v(0)\tilde{v}(t)$ and integrate with respect to $x,y,\tilde{x},\tilde{y}$.

- Using our approach we get analytic results for the VAF.
  We recover the results of Jepsen, Lebowitz, Sykes and Percus. Our approach is much simpler than the earlier approaches.
  Analytic results obtained for the long time behaviour where finite size effects become important.
  [A. Roy, O. Narayan, A. Dhar, S. Sabhapandit, JSP (2012)]

Equal mass HP gas



Simulation results —
also reproduced by exact analysis.

Comparision between harmonic chain (HC) and hard particle gas (HPG):

1. Both integrable models
2. Both diffusive at intermediate time scales.
3. VAF — $\sin(\omega_0 t)/t^{1/2}$ in HC and $\sim -1/t^3$ in HPG.
4. Finite size effects very different — MSD keeps oscillating in HC, saturates to equilibrium value for HPG.

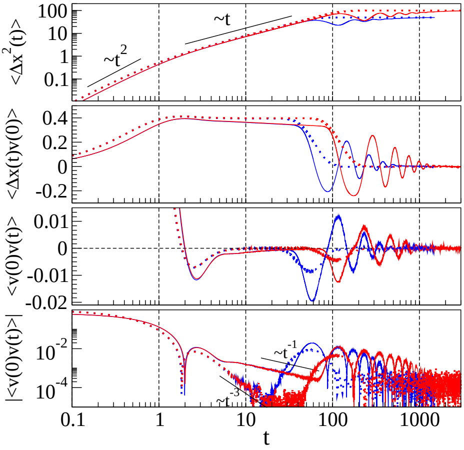
Alternate mass HP gas

- What about the case when alternate particles have different masses? From momentum and energy conservation we have

$$
\begin{aligned}
v_l' &= \frac{(m_l - m_{l+1})}{(m_l + m_{l+1})} v_l + \frac{2m_{l+1}}{(m_l + m_{l+1})} v_{l+1} \\
v_{l+1}' &= \frac{2m_l}{(m_l + m_{l+1})} v_l + \frac{(m_{l+1} - m_l)}{(m_l + m_{l+1})} v_{l+1} \ .
\end{aligned}
$$

- In this case the mapping to non-interacting particles breaks down and we do not have any exact results — Simulation results.

Hard particle gas- simulation results



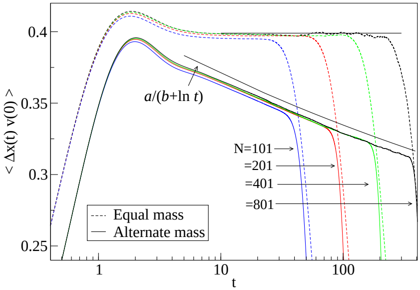
Alternate mass HPG (solid lines) compared with equal mass HPG.
$N = 101$ (blue) and $N = 201$ (red) particles, density $\rho = 1$ and $k_B T = 1$. Alternate particles have masses 1.5 and 0.5.

Note:

VAF for AM-HPG is close to $\sim -1/t$.

Oscillations at large times (sound waves).

Hard particle gas- behaviour of $D(t)$.

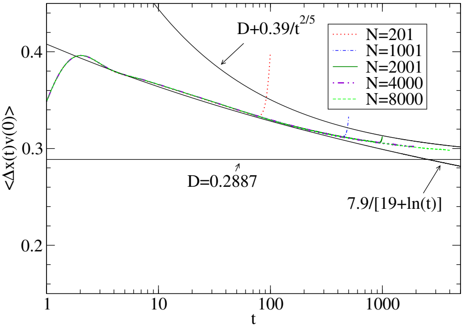


Plot of $D(t) = \langle \Delta x(t) v(0) \rangle$ for the alternate mass gas for various system sizes. We see a logarithmic decay of the diffusion constant.
Dashed line shows saturation to the expected Jepsen value $1/\sqrt{2\pi} \approx 0.4$ for equal mass HPG.

A Roy, O. Narayan, A. Dhar and S. Sabhapandit, JSP (2012).

Contradicts results of mode-coupling theory (H van Beijeren) which predicts —
$D(t) = D + 0.39/t^{2/5}$ with $D = k_B T/(2nc) = 0.2887$.

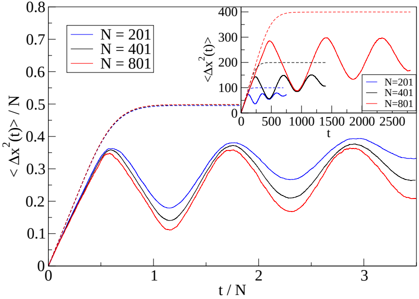
Hard particle gas - behaviour of $D(t)$ [Latest simulations !]



Data seems to approach Beijeren formula from mode-coupling theory.

Slow decay to a finite asymptotic diffusion constant $D = k_B T/(2nc)$, where c is the sound speed.

Note that diffusion constant is independent of mass ratio and depends only on the average density. For unit density and temperature, $D = 1/\sqrt{2\pi} = 0.3989...$ for equal mass case and this changes to $D = 1/(2\sqrt{3}) = 0.2886...$ even if the masses are different by arbitrarily small amounts.



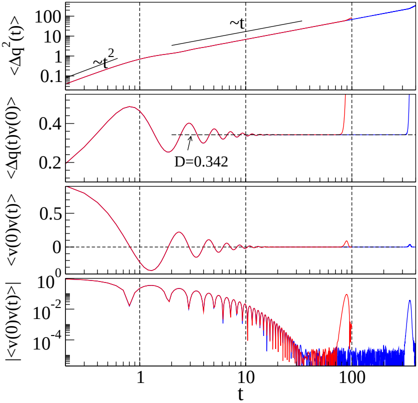
MSD as a function of time for three system sizes $N = 201, 401, 801$.

Equilibrium saturation value for alternate mass and equal mass HPG are the same but the approach to this is very different.

Fermi-Pasta-Ulam chain: Short time behaviour

Hamiltonian given by

$$H = \sum_{l=1}^{N} \frac{m}{2}\dot{q}_l^2 + \sum_{l=1}^{N+1}\left[\frac{k}{2}(q_l - q_{l-1})^2 + \frac{\nu}{4}(q_l - q_{l-1})^4\right]$$

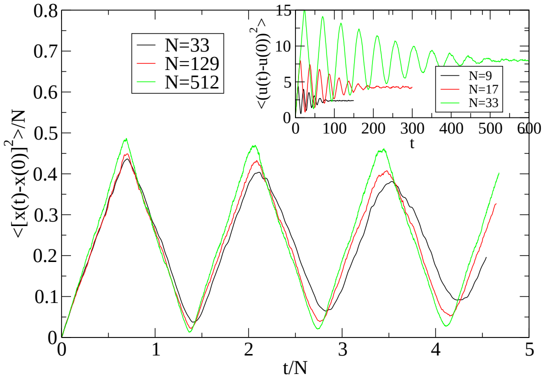


We see that there is a fast convergence of $D(t)$ to the expected diffusion constant $D = k_B T/(2nc) = 0.342$

Sound speed c can be calculated from one-dimensinal hydrodynamics theory (H. Spohn, 2013).

VAF $\sim \sin(\omega_0 t)e^{-At}$.
Compare with HC ($\sim \sin(\omega_0 t)/t^{1/2}$).

Fermi-Pasta-Ulam chain: Long time behaviour



Oscillations with time period N/c and eventual saturation to equilibrium value $\langle [\Delta x(t)]^2 \rangle \to 2[\ \langle x^2 \rangle - \langle x \rangle^2\ ] \sim N$ (unlike harmonic case).

Sound waves with noise and dissipation

Consider hydrodynamic description of the one-dimensional chain in terms of sound modes which are acted on by **momentum-conserving noise and dissipation**.

$$m\ddot{q}_l = -k(2q_l - q_{l+1} - q_{l-1}) - \gamma(2\dot{q}_l - \dot{q}_{l+1} - \dot{q}_{l-1}) + (2\xi_l - \xi_{l+1} - \xi_{l-1}) \ .$$

For equilibration we require

$$\langle \tilde{\xi}_p(t)\, \tilde{\xi}_{q'}(t') \rangle = \frac{2\gamma k_B T}{\omega_p^2} \delta(t-t')\, \delta_{q,q'} \ .$$

Solving the linear equations we get the following correlations for the middle particle:

$$\begin{aligned} \langle q(t) v(0) \rangle &= \frac{2k_B T}{m(N+1)} \sum_{s=1,3,\ldots} \frac{1}{\beta_p} e^{-\alpha_p t} \sin(\beta_p t) \ , \\ \langle v(t) v(0) \rangle &= \frac{2k_B T}{m(N+1)} \sum_{s=1,3,\ldots} e^{-\alpha_p t} \left[\cos(\beta_p t) - \frac{\alpha_p}{\beta_p} \sin(\beta_p t) \right] \ . \end{aligned}$$

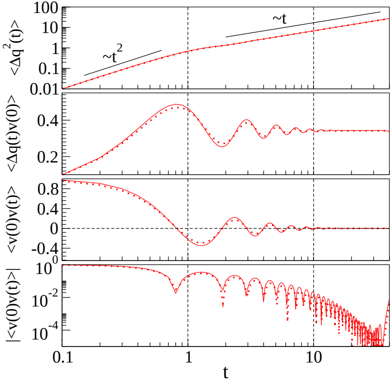
Diffusion constant:

$$D = \lim_{t\to\infty} \langle q(t) v(0) \rangle = \frac{k_B T}{mc\pi} \int_0^\infty dx \frac{\sin x}{x} = \frac{k_B T}{2\rho c} \ .$$

Sound waves with noise and dissipation – comparision with FPU data

Comparision of the predictions of effective model with simulation results of FPU chain ($N = 65$).

γ is the only fitting parameters. k fixed from FPU speed of sound (Spohn, 2014).



Very good agreement between model and actual FPU chain data.

The decay of the VAF is as $\sim sin(\omega_0 t)e^{-\alpha t}/t^{1/2}$.

Velocity autocorrelation function

Effective model gives

$$\langle v(t)v(0)\rangle \quad = \quad \frac{2k_BT}{m(N+1)} \sum_{s=1,3,\dots} e^{-\alpha_p t} \left[\cos(\beta_p t) - \frac{\alpha_p}{\beta_p} \sin(\beta_p t)\right] .$$

For $N \to \infty$, asymptotic (large t) analysis gives

$$\langle v(t)v(0)\rangle \sim \frac{e^{-\gamma t} \sin(\omega_0 t)}{t^{1/2}}.$$

This approach is similar to harmonization technique used for **interacting Brownian particles** . [Lizana, Barkai etal, PRE (2010)] — There one gets

$$\langle \Delta x^2(t)\rangle = \frac{2}{\pi^{1/2}} \frac{k_B T}{\rho c} \left(\frac{t}{\gamma/m}\right)^{1/2} .$$

Identity-exchange dynamics

- Definition of dynamics: we define the interacting problem by starting with the non-interacting trajectories and interchanging particle labels whenever two trajectories cross.
- Models of (i) hard particle gas starting from equilibrium velocity distribution and (ii) reflecting Brownian particles both fall in the above classification.
- In both these cases, single particle dynamics is described by the Gaussian propagator

$$G(y,t|x,0) = \frac{1}{\sqrt{2\pi\sigma_t^2}} \exp\left(-\frac{(y-x)^2}{2\sigma_t^2}\right).$$

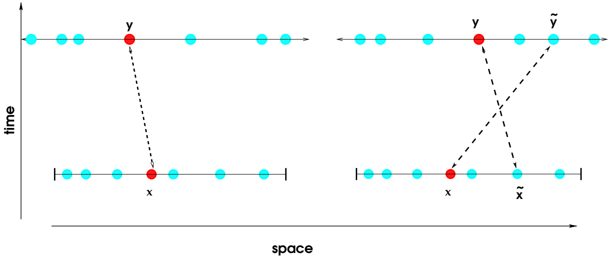
$\sigma_t = \bar{v}t$ for HPG and $\sigma_t = \sqrt{2Dt}$ for BM.

- It is easy to compute properties of the interacting system by mapping to non-interacting dynamics.

EXAMPLE: - computing joint distribution of tagged particule $P(x,0;y,t)$.

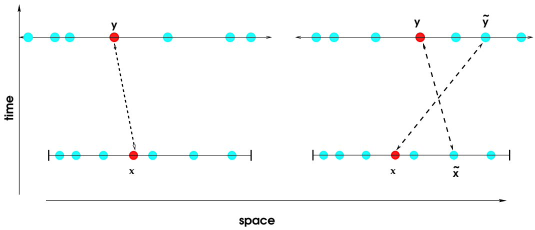
Mapping to non-interacting problem

In the noninteracting picture, there are two possibilities:
(i) the middle particle at $t = 0$ is still the middle particle at time t.
(ii) a second particle has become the middle particle at time t.



We need to sum over these two processes.

Mapping to non-interacting problem



- $P_{(1)}(x,0;y,t) = \rho\, G(y,t|x,0)\, F_{1N}(x,y,t)$.
  $F_{1N}(x,y,t)$ is the probability that there are an equal number of particles to the left and right of x and y at $t=0$ and t respectively.
- $P_{(2)}(x,0;y,t) = \rho^2 \int_{-\infty}^{\infty} d\tilde{x} \int_{-\infty}^{\infty} d\tilde{y}\, G(\tilde{y},t|x,0)\, G(y,t|\tilde{x},0)\, F_{2N}(x,y,\tilde{x},\tilde{y},t)$.
  $F_{2N}(x,y,\tilde{x},\tilde{y},t)$ is the probability that there are an equal number of particles on both sides of x and y at $t=0$ and t respectively, given that there is a particle at $\tilde{x}$ at time $t=0$, and a particle at $\tilde{y}$ at time t.
- $P(x,0;y,t) = P_{(1)}(x,0;y,t) + P_{(2)}(x,0;y,t)$.

Large deviation functions of TPD in single-file systems

[C. Hegde, A. Dhar, S. Sabhapandit, PRL (2014)]

- The functions F_{1N} and F_{2N} can be obtained using combinatorial arguments. Hence we can obtain the exact joint PDF.

- The joint PDF gives the full PDF of the tagged particle displacement.

- Final result:- PDF has the large deviation form

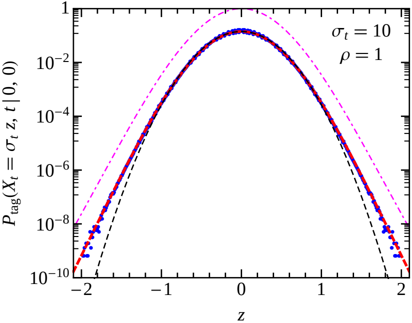
$$P_{\mathrm{tag}}(X, t|0,0) \sim e^{-\rho \sigma_t I(X/\sigma_t)} ,$$

where the large deviation function (LDF) is given exactly by

$$I(z) = 2Q(z) - \left[4Q^2(z) - z^2\right]^{1/2}, \quad Q(z) = \frac{e^{-z^2/2}}{\sqrt{2\pi}} + \frac{z}{2}\,\mathrm{erf}\left(z/\sqrt{2}\right).$$

Earlier treatment — C. Rödenbeck, J. Kärger, and K. Hahn (1998)—from N-particle propagator.

Large deviation function



- Can compute leading correction to LDF. This is improtant for numerical comparision.
- Can also compute cumulant generating function and all cumulants. No closed-form expression.

Other results

- Comparision with Macroscopic Fluctuation Theory result.
  [P. Krapivsky, K. Mallick, T. Sadhu, PRL (2014)].

- Two time correlations can be computed —
  From MFT [P. Krapivsky, K. Mallick, T. Sadhu, JSP (2015)].

  From non-interacting system mapping [T. Sadhu and B. Derrida, JSM (2015)].

  Shows that tagged particle motion is non-Markovian.

- Two-particle joint distributions can be computed using the same method.

  [Sabhapandit and Dhar, JSM (2015)]

Conclusions

- Effect of non-integrable interactions on tagged particle diffusion was studied. (Can chaotic motion give rise to subdiffusive behaviour ?)
- Tagged particle motion in Hamiltonian systems is probably diffusive in all cases.
  Diffusion constant known exactly for equal mass hard particle model, harmonic chain.
  Diffusion constant from linearized hydrodynamic equations is $D = k_B T/(2\rho c)$. The speed of sound in terms of parameters of microscopic models is known [Spohn (2013)]. Very accurate in many cases, less so in some.
- For the alternate mass case, approach to asymptotic behaviour seems to be slow
  — Mode coupling theory (Beijeren)
  For the FPU case we get a fast approach to the expected asymptotic diffusion constant.
- The velocity autocorrelation function can have a wide range of asymptotic behaviour including power-law decay, oscillatory decay, as well as exponential decay.
- The approach to equilibration and finite-size effects are also very different in different models.
- Proposed a powerful method for exact computations in class of single-file systems.