

Many Particle Systems

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Introduction

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Master Equation

Second Quantization

SDE

Its Form

Solving the SDE

Results

Numerically

The Future

The Classical Problem

- ▶ Classical rate equations fail in the limit of relatively small finite particle populations.
- ▶ Our investigations start with the reaction $A + A \rightarrow A$.
- ▶ We only have one species of particle whose population after some time T_f will reach 1.

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- ▶ $\frac{dc}{dt} = -\kappa c^2$
- ▶ c is the mean particle population and κ is the rate coefficient
- ▶ In the “thermodynamic limit” i.e where populations are large and fluctuations are relatively small; $\langle \phi^2 \rangle \approx \langle \phi \rangle^2$, $c = \langle \phi \rangle$.

The Master Equation

- ▶ First we must write a master equation for this reaction.
- ▶
$$\frac{dP(N,t)}{dt} = \frac{\kappa}{2V} [(N+1)NP(N+1,t) - N(N-1)P(N,t)]$$

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- ▶ Finally using path integral formalism we are able to extract a Stochastic Differential Equation (SDE).

Our SDE from the black box

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- ▶ Where we are interested in $\langle \Phi(t) \rangle$.

Solving the SDE

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- ▶ Analytically: Here we use Itô calculus to construct a solution.
- ▶ Numerically: Using a sequence of random numbers to create a *Wiener* process and implementing it in an iterative method. We then average over a large number of *runs*.

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$$\Phi(t) = \frac{\Phi_0 \exp(\kappa t + i\sqrt{2\kappa}W(t))}{1 + \kappa \Phi_0 \int_0^t \exp(\kappa s + i\sqrt{2\kappa}W(s)) ds}$$

Numerically

- ▶ A Wiener process can be defined as such, $W(0) = 0$ w.p.1, $E(W(t)) = 0$ and finally $Var(W(t) - W(s)) = t - s$

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- ▶ We can construct something very similar by dividing our time interval into equal length sub intervals. $\frac{t_i}{N}$
- ▶ We then generate a list of gaussian random numbers, $\{X_1, X_2, \dots, X_N\}$ with $\mu = 0$.
- ▶ Then we sum these numbers such that $S_N(t_n^{(n)}) = (X_1 + X_2 + \dots + X_n)\sqrt{\Delta t}$

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- ▶ $d\Phi(t) = -\kappa\Phi^2(t)dt + i\sqrt{(2\kappa)}\Phi(t)dW$
- ▶ Where $dW = \eta dt$.

Single Projection of $\text{Re}(\Phi(t))$

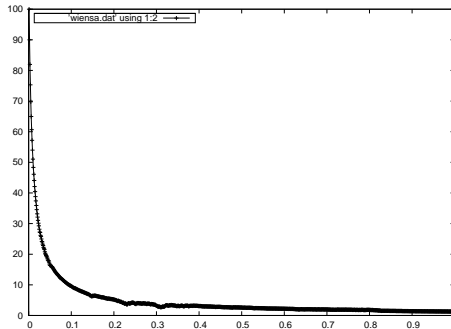


Figure: The real part of a single realisation of the solution to the SDE

Single Projection of $\text{Im}(\Phi(t))$

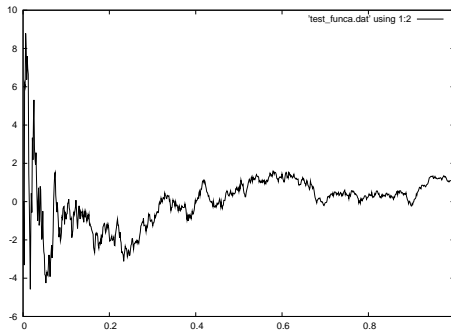


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$$\text{Re}(\langle \Phi(t) \rangle)$$

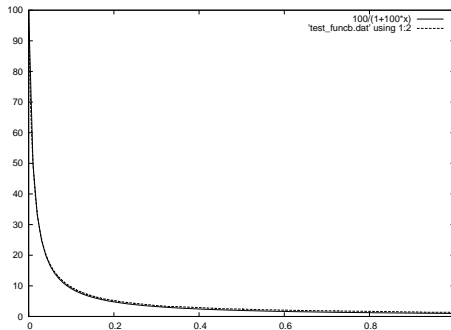


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$\text{Im}(\langle \Phi(t) \rangle)$

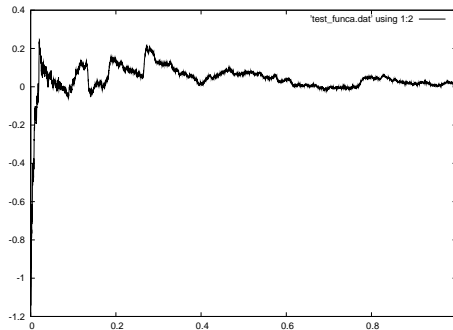


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What I would like to move onto next;

- ▶ To calculate a reaction where a single “super” dust particle forms.



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- ▶ To calculate a reaction where a single “super” dust particle forms.
- ▶ Is it possible to show that $\text{Im}(\langle \Phi(t) \rangle) = 0$ for all time?