Robotics and Autonomous Systems 96 (2017) 15–25

Contents lists available at ScienceDirect

Robotics and Autonomous Systems

journal homepage: www.elsevier.com/locate/robot

Simple exclusion model applied to nano-robots

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HIGHLIGHTS

- Motion of robot links attached to the lattice sites of a simple exclusion process.
- Approximate mean and covariance propagation equations for particle number at sites.
- Average Lagrangian of the system of links attached to the occupied sites interacting.
- Quantization of the link motion via the Schrodinger wave function is studied.
- Complete plots of the density and covariance profile of the exclusion process.

ARTICLE INFO

Article history:
Received 27 April 2016
Received in revised form 5 May 2017
Accepted 23 May 2017
Available online 13 October 2017

Keywords:
Markov process
Poisson process
Simple exclusion model
Robot link kinetic energy
Mean and covariance propagation
Euler–Lagrange equation
Non-linear diffusion equation
Nano-robot
Schroedinger equation
Fluid density and velocity field

ABSTRACT

The motion of robot links attached to the lattice sites of a simple exclusion process in $\mathbb{Z}_N^3$ is described. Approximate mean and covariance propagation equations for the particle number at the sites is derived. The average Lagrangian of the system of links attached to the occupied sites interacting with each other on a pair wise basis via potential dependent on the lattice sites and the link orientations at the two sites is setup. Complete plots of the density and covariance profile of the exclusion process are generated based on Poisson process simulation. Plots of the link angles are also generated. Quantization of the link motion via the Schroedinger wave function is studied.

1. Introduction

We consider a simple exclusion process as in [1] involving particles distributed over the large $\mathbb{Z}_N^3$ with particles jumping from one occupied sites to unoccupied sites in accordance with a Poisson process clock with rates dependent on the location of the sites. Such a process $\{\eta_t(x) \ : \ x\epsilon\mathbb{Z}_N^3\}_{t\geq 0}$ determines a Markov process whose generator can easily be calculated [1]. Now each particle in an occupied site x is replaced by a robot link whose direction angles $(\theta_t(x), \phi_t(x))$ at time t determine its kinetic energy and potential energy of interaction with a link at another occupied site y specified by angles $(\theta_t(y), \phi_t(y))$.

Two kinds of model are proposed to study the dynamics of $(\theta_t(x), \phi_t(x))$. In the first, these angles are regarded as deterministic process and the average Lagrangian of the system is calculated by averaging over functions of the exclusion-process $\{\eta_t(x)\}$. The Euler–Lagrange equations for the angles $\{\theta_t(x), \phi_t(x)|x\epsilon\mathbb{Z}_N^3\}$ are then set up. In the second model, we do not take the probabilistic average of the Lagrangian but rather work with the random Lagrangian and set up the Euler–Lagrangian differential equation for the process $(\theta_t(x), \phi_t(x))$, $x\epsilon\mathbb{Z}_N^3$, $t \geq 0$ using the random Lagrangian. This yields us differential equation for $\theta_t(x), \phi_t(x)$ with random process coefficients coming as functions of the exclusion process $\{\eta_t(x)\}$. we then set up an approximate analysis of these equations. In the former case, we derive approximate mean and covariance propagation equation for the exclusion process $\eta_t(x)$. The average $\mathbb{E}\eta_t(x) = \rho_t(\frac{x}{N})$ gives us the particle density at the site x while the covariances $C_t(\frac{x}{N}, \frac{y}{N}) = \mathbb{E}(\delta\eta_t(x)\delta\eta_t(y))$ gives us fluctuations in the particle density at each site and the correlations in the fluctuations at different sites. Here $\delta\eta_t(x) = \eta_t(x) - \rho_t(\frac{x}{N})$. Approximate mean propagation and covariance propagation equation for $\rho_t(\frac{x}{N})$ and $C_t(\frac{x}{N}, \frac{y}{N})$ are derived from the Poisson driven

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http://dx.doi.org/10.1016/j.robot.2017.05.009
0921-8890/

stochastic differential equation for $\eta_t(x)$. These approximate mean and covariance propagation equations are used in the former Lagrangian by expanding functions of $\eta_t(x)$ around its mean $\rho_t(\frac{x}{N})$. Certain assumptions regarding the interaction potential energies between particles at two sites x and y i.e. $V(\theta_t(x), \phi_t(x), \theta_t(y), \phi_t(y))$ are made like assuming $\frac{\|y-x\|}{N}$ is small for significant interactions. This causes

$$\begin{aligned} &V(\theta_t(x), \phi_t(x), \theta_t(y), \phi_t(y)) \\ &\quad \approx V(\theta_t(x), \phi_t(x), \theta_t(x) + (y-x)\theta_t'(x), \phi_t(x) + (y-x)\phi_t'(x)), \quad (1) \end{aligned}$$

i.e. average Lagrangian depends only on $\theta_t, \phi_t, \theta_t', \phi_t', \dot{\theta}_t, \dot{\phi}_t$ and non-linear wave equations for θ_t, ϕ_t can be obtained in the limit $\frac{|y-x|}{N} \xrightarrow[N\to\infty]{} 0$.

In the latter model, we also need to set mean and covariance propagation equations for the angles $\theta_t(x), \phi_t(x)$ as these quantities now become stochastic processes driven by the exclusion process. Further we may also assume that the Poisson jump rate from one site x to another site y depends on the angles $\theta_t(x), \phi_t(x)$. We thus need to set up approximate mean and covariance propagation equations for

$$\left\{ \begin{bmatrix} \eta_t(x) \\ \theta_t(x) \\ \phi_t(x) \end{bmatrix}, x \epsilon \mathbb{Z}_N^3 \right\}. \quad (2)$$

We do not perform the entire analysis for this case. The final section of the analysis part of this paper is to study quantization of the system described by the average Lagrangian. This is achieved by assuming that the kinetic energy of each link in an occupied site is a quadratic function of $(\dot{\theta}_t(x), \dot{\phi}_t(x))$ and perform a Legendre transformation to express the average Hamiltonian as quadratic function of the canonical moment $(p_{\theta x}(t), p_{\phi x}(t)), x\epsilon\mathbb{Z}_N^3$. We then set up the Schroedinger equation by replacing $p_{\theta x}(t)$ with $\iota\frac{\partial}{\partial\theta(x)}$ and $p_{\phi x}(t)$ with $\iota\frac{\partial}{\partial\phi(x)}$.

The simulation part consists of MATLAB plots of the exclusion process $\eta_t(x)$ at each site $x = 1, 2, 3, \dots, N$ assuming nearest neighbour interactions only, i.e.

$$\begin{aligned} d\eta_t(x) = &\sum_{y=1, y\neq x}^{N} \eta_t(y)(1-\eta_t(x))dN_t(y,x) \\ &- \eta_t(x)(1-\eta_t(y))dN_t(x,y), \end{aligned} \quad (3)$$

where $N_t(x, y), x \neq y$ are $N(N-1)$ independently generated Poisson process. For a simple case with $N = 10$, we also display plots of the link angles $\theta_t(x), \phi_t(x), 1 \le x \le 10, t \ge 0$.

The behaviour of tagged particles in simple exclusion models has been studied in Quastel, Kipnis and Varadhan [1,2]. Here the state space of the Markov process is $\{0,1\}^{\mathbb{Z}_N^d}$ or if p colours are included as in Quastel [1], the state space is $\{0, 1, 2, \dots, p-1\}^{\mathbb{Z}_N^d}$. The hydrodynamic scaling limit i.e. the limiting densities of the coloured particles satisfy non-linear partial differential equation's in the scaling limit. These have been derived in Quastel [1]. Here we go a step further by assuming that at each occupied site is located a link whose angles can vary with time and in some cases, the transition probability of a link from one site to the other depends on this orientation angle. In the scaling limit, fluid particles are located every where and yet transitions of links can take place in the sense of ensemble averages. This has been the objective of our work. Thus links present at two different lattice sites can undergo mutual transitions dependent upon the relative angular orientation of the links. This happens for example in electro-magnetics. When the links carry currents which produce magnetic fields which interact with the currents in other links. In other words we superpose a link structure on the simple exclusion model.

Kipnis and Varadhan [2] derive a central limit theorem for tagged particles in simple exclusion and we can generally consider based on this, links attached to the tagged particles executing diffusion processes and interacting according to their angular orientation. Such problems will be studied in a future paper.

In Jang, et al. [3] motion of a micro-robot moving in a microfluidic system controlled by em fields is discussed. This problem is very similar to our if we assume that the fluid consists of particles which can diffuse. In fact, using the asymmetric simple exclusion model Kipnis, et al. [4] derive an equation of the form

$$\frac{\partial\rho}{\partial t} = \nabla.(D\nabla\rho) + \nabla.(b\rho(1-\rho)), \quad (4)$$

in the scaling limit which is a non-linear diffusion equation. Varadhan [5] also talks about deriving the fundamental fluid dynamical equations by perturbing Hamiltonian systems with noise. In this case, they also obtain partial differential equations for the velocity field. Even in (4), if we assume a robot located at site x interacting via em fields with a robot at site y, then we would obtain our model for the angular orientations of our robot.

The motor of robot in a microfluidic system as in Wang, et al. [3] can be used in medical applications wherein the fluid is blood.

Let $v(t, r)$ denote the fluid velocity field. Then the kinetic energy of two robots moving along two different fluid trajectories is of the form

$$\begin{aligned} &T_1(\theta_1, \phi_1, \dot{\theta}_1(t), \dot{\phi}_1(t)) + T_2(\theta_2, \phi_2, \dot{\theta}_2(t), \dot{\phi}_2(t)) \\ &\quad + \frac{1}{2}m_1|\dot{r_1}(t)|^2 + \frac{1}{2}m_2|\dot{r_2}(t)|^2, \end{aligned} \quad (5)$$

where $\dot{r_1}(t) = v(t, r_1(t)), \dot{r_2}(t) = v(t, r_2(t))$ and the potential energy of interaction between the two robots is of the form

$$V(r_1(t), r_2(t), \theta_1, \phi_1, \theta_2, \phi_2). \quad (6)$$

So if the fluid velocity field is known, we can set up the Euler–Lagrange equation of the system.

In the simple exclusion model for the fluid, we may also take into account the translational velocity of motion in the kinetic energy, via the method discussed in the paper, i.e. the average velocity of a particle moving from site x to site y is

$$\begin{aligned} v(t, x, y) &= \mathbb{E}\left[\eta_t(x)(1-\eta_t(y))\frac{(y-x)}{dt}dN_t(x,y)\right] \\ &= p(x,y)(y-x)\mathbb{E}(\eta_t(x)(1-\eta_t(y))). \end{aligned} \quad (7)$$

Further, Quastel, et al. [6] have considered the problem of determining the Large deviation rate functional for the empirical density. Specifically they first consider a symmetric simple exclusion process, and write down the Radon–Nikodym derivative of the probability law of this process w.r.t. the same process perturbed by weak asymmetry. They use this to compute the relative entropy between the two processes and minimize this relative entropy w.r.t the asymmetric perturbation of the jump probability subject to constant "drift". The resulting expression is used to arrive at a nice formula for the rate function. We can hope to generalize this to the case of interacting links with the joint rate function for the empirical density and the link angles.

In Tabak and Yesilyurt [7], the motion of a 3-D rigid body, or more precisely a two link helical swimmer in a fluid has been studied. The fluid resistance force on the rigid body has been modelled as being proportional to the 3-D velocity vector with a damping force matrix being the velocity damping coefficient. Explicit formulas for this matrix are obtained in terms of the rotation matrix between the local fluid frame and the 3-d body frame.

Further the motion of the rigid body in the fluid causes the fluid velocity field to change. This is modelled by the Navier–Stokes equation in the rotating frame of the rigid body. This model can be incorporated in our paper by considering an array of rigid bodies moving in a fluid, with a rigid body making a transition from one