An exact sampling scheme for Brownian motion in the presence of a magnetic field

Mini P. Balakrishnan, M. C. Valsakumar and P. Rameshan

1 Department of Physics, University of Calicut, Calicut University PO, Pin 673635, India
2 Materials Science Division, IGCAR, Kalpakkam, Pin 603102, India

(Dated: March 22, 2022)

Langevin equation pertinent to diffusion limited aggregation of charged particles in the presence of an external magnetic field is solved exactly. The solution involves correlated random variables. A new scheme for exactly sampling the components of the position and velocity is proposed.

I. INTRODUCTION

The diffusion limited aggregation (DLA) model and some of its variants have been used to model pattern formation in diverse contexts such as electrochemical deposition, dissolution and erosion of porous media, gelation, fracture, dielectric breakdown etc. These patterns, in general, have a fractal structure and the study of DLA clusters have resulted in the understanding of various aspects of fractals such as fractal dimension, multifractality and the scaling laws. The insight obtained from the analysis of DLA clusters has led to the application of this model to the study of the scaling behavior of two-dimensional quantum gravity. Yet a complete theoretical understanding of DLA has not been achieved to date. Recently, a few groups have carried out experimental investigation of the influence of an external magnetic field on DLA of charged particles. They observed a bending of the branches of the DLA cluster, which could be attributed to the Lorentz force, as well as a conspicuous change in the morphology of the clusters with increase in the strength of the magnetic field.

II. SOLUTION OF LANGEVIN EQUATION IN THE PRESENCE OF MAGNETIC FIELD

Consider the Langevin equation describing the Brownian motion of a charged particle of unit mass and charge $q$, in presence of a magnetic field $\vec{B}$ along the z-direction

$$\frac{d}{dt}\vec{r}(t) = \vec{v}(t)$$

$$\frac{d}{dt}\vec{v}(t) + \gamma\vec{v}(t) - q\vec{v}(t) \times \vec{B} = \vec{\eta}(t)$$

In the above equation, $\vec{\eta}(t) = \langle \eta_1(t) \rangle \delta(t - t')$ is a Gaussian white noise of zero mean and its components satisfy the normalization condition

$$\langle \eta_i(t) \eta_j(t') \rangle = 2A\delta_{ij}\delta(t - t')$$

Since the magnetic field is oriented along the z-direction, it affects the motion in the x and y directions only. Defining

$$X = x + iy, \quad V = v_1 + iv_2, \quad \Gamma = \gamma + i\omega, \quad \eta = \eta_1 + i\eta_2$$

we get

$$\frac{d}{dt}X = V$$

$$\frac{d}{dt}V + \Gamma V = \eta(t)$$

The formal solution is given by

$$V(t) = e^{-\Gamma t}V(0) + \int_0^t e^{-\Gamma(t-t_1)}\eta(t_1) \, dt_1$$

$$X(t) - X(0) = \frac{1}{\Gamma} \left( (1 - e^{-\Gamma t})V(0) + \left[ \int_0^t \eta(t_1) \, dt_1 - \int_0^t e^{-\Gamma(t-t_1)}\eta(t_1) \, dt_1 \right] \right)$$

Using the above formal solution, we can immediately obtain $x(t), y(t)$ by taking the real and imaginary parts of $X(t)$. $v_1(t)$ and $v_2(t)$ can also be obtained in a similar fashion. The two time correlation functions of $v_1(t)$ and $v_2(t)$ are given by

$$\langle v_1(t)v_1(t') \rangle = \left( \frac{A}{2} \right) e^{-\gamma|t-t'|} \cos(\omega|t-t'|)$$
\[
\langle v_2(t)v_2(t') \rangle = \langle v_1(t)v_1(t') \rangle
\]  
(10)
\[
\langle v_1(t)v_2(t') \rangle = \left(\frac{A}{\gamma} \right) e^{-\gamma|t-t'|} \sin(\omega(t-t'))
\]  
(11)
The other correlation functions can also be calculated easily.

The interesting point is that unlike in the case of the motion without the magnetic field, now the components \(v_1(t)\) and \(v_2(t')\), of the velocity, are correlated. But, the second moment \(\langle v_1(t)^2 \rangle\), of each of the components of the velocity, has the same value \(A/\gamma\) as in the case of zero magnetic field. This can be easily understood once we recognize that \(\langle v_1(t)^2 \rangle\) is twice the kinetic energy and that does not change by application of a magnetic field. However, \(\langle x(t)^2 \rangle\) and \(\langle y(t)^2 \rangle\) asymptotically (i.e., as \(t \to \infty\)) tend to \(\frac{2A}{\gamma^2+\omega^2} t^2\) so that the diffusion coefficient \(D = \frac{A}{\gamma^2+\omega^2}\) decreases with increasing magnetic field.

In the numerical simulations we will be interested in getting realizations of \(x(t)\), \(y(t)\), etc. at discrete instants of time \(t_j = j \times \tau\). We have developed such a scheme that is valid for arbitrary values of \(A\), \(\omega\), \(\gamma\) and \(\tau\).

Define
\[
x_j = x(t_j), \quad y_j = y(t_j), \quad X_j = x_j + iy_j
\]  
(12)
\[
\psi_j = \int_0^\tau du \, \eta (j \tau + u)
\]  
(13)
\[
\phi_j = \int_0^\tau du \, e^{-\Gamma(\tau-u)} \eta (j \tau + u)
\]  
(14)

\[
\psi_j = \sum_{l=0}^{j-1} \psi_l
\]  
(15)
\[
\phi_j = \sum_{l=0}^{j-1} e^{-(j-l-1)\tau \Gamma} \phi_l
\]  
(16)

We can then write
\[
X_j = \frac{1}{\Gamma} \left[ (1 - e^{-\Gamma \tau}) V(0) + \psi_j^{(t)} - \phi_j^{(t)} \right]
\]  
(17)

We can perform the numerical simulations if we can reliably sample \(\psi_j\) and \(\phi_j\). Since \(\psi_j\) and \(\phi_j\) depend on \(\eta\) in the interval \([j \tau, (j+1) \tau]\) alone, and since the \(\{\eta_l\}\) are delta-correlated, we can immediately see that \(\langle \psi_j \psi_j' \rangle\) and \(\langle \phi_j \phi_j' \rangle\) vanish when \(j \neq j'\). However, \(\psi_j\) and \(\phi_j\) are correlated. Therefore it is important to evolve a procedure to sample these correlated random variables.

It is convenient to work with the following real random variates:
\[
\psi_{jR} = \Re(\psi_j) = \int_0^\tau du \, \eta_1(j \tau + u)
\]  
(18)
\[
\psi_{jI} = \Im(\psi_j) = \int_0^\tau du \, \eta_2(j \tau + u)
\]  
(19)
\[
\phi_{jR} = \Re(\phi_j) = \int_0^\tau du \, e^{-\gamma(\tau-u)} [\cos(\omega(\tau-u)) \eta_1(j \tau + u) + \sin(\omega(\tau-u)) \eta_2(j \tau + u)]
\]  
(20)
\[
\phi_{jI} = \Im(\phi_j) = \int_0^\tau du \, e^{-\gamma(\tau-u)} [-\sin(\omega(\tau-u)) \eta_1(j \tau + u) + \cos(\omega(\tau-u)) \eta_2(j \tau + u)]
\]  
(21)

In the above equations, \(\Re(z)\) and \(\Im(z)\) are the real and imaginary parts of the complex number \(z\). Since \(\psi_j\) and \(\phi_j\) are Gaussian random variates of zero mean, the knowledge of their covariance is adequate for describing them. They are given below:

\[
\langle \psi_{jR} \psi_{j'R} \rangle = 2A \delta_{j,j'}, \quad \langle \psi_{jI} \psi_{j'I} \rangle = 2A \delta_{j,j'}, \quad \langle \psi_{jR} \psi_{j'I} \rangle = 0
\]  
(22)
\[
\langle \phi_{jR} \phi_{j'R} \rangle = \frac{A}{\gamma} (1 - e^{-2\gamma \tau}) \delta_{j,j'}, \quad \langle \phi_{jI} \phi_{j'I} \rangle = \frac{A}{\gamma} (1 - e^{-2\gamma \tau}) \delta_{j,j'}, \quad \langle \phi_{jR} \phi_{j'I} \rangle = 0
\]  
(23)
\[
\langle \phi_{jR} \psi_{j'R} \rangle = \frac{2A}{\gamma^2 + \omega^2} \left[ (1 - e^{-\gamma \tau} \cos(\omega \tau)) \eta_1(j \tau + u) + \omega e^{-\gamma \tau} \sin(\omega \tau) \right] \delta_{j,j'}
\]  
(24)
\[
\langle \phi_{jI} \psi_{j'I} \rangle = \frac{2A}{\gamma^2 + \omega^2} \left[ \omega(1 - e^{-\gamma \tau} \cos(\omega \tau)) - e^{-\gamma \tau} \sin(\omega \tau) \right] \delta_{j,j'}
\]  
(25)
\[
\langle \phi_{jI} \psi_{j'R} \rangle = -\langle \phi_{jR} \psi_{j'I} \rangle, \quad \langle \phi_{jI} \psi_{j'I} \rangle = \langle \phi_{jR} \psi_{j'R} \rangle
\]  
(26)

Our aim is to provide a scheme for sampling \(\psi_{jR}, \psi_{jI}, \phi_{jR}\) and \(\phi_{jI}\) that is consistent with the above equations. We propose to achieve this by expressing \(\psi_{jR}, \psi_{jI}, \phi_{jR}\) and \(\phi_{jI}\) as sums of \(n\) identically distributed Gaussian random variates.
random variables \((p_{j1}, p_{j2}, ..., p_{jn})\) with zero mean and unit variance in the following manner:

\[
\psi_{jR} = \sqrt{2A} \sum_{l=1}^{n} \alpha_l p_{jl} \quad (27)
\]

\[
\psi_{jl} = \sqrt{2A} \sum_{l=1}^{n} \beta_l p_{jl} \quad (28)
\]

\[
\phi_{jR} = \sqrt{A(1 - e^{-2\gamma r})} \sum_{l=1}^{n} \epsilon_l p_{jl} \quad (29)
\]

\[
\phi_{jl} = \sqrt{\frac{A(1 - e^{-2\gamma r})}{\gamma}} \sum_{l=1}^{n} \nu_l p_{jl} \quad (30)
\]

The substitution of the above results in equations (27)–(30) gives 10 constraints that the parameters \(\alpha_l, \beta_l, \epsilon_l\) and \(\nu_l\) should satisfy.

\[
\begin{align*}
\sum_{l=1}^{n} \alpha_l^2 &= 1, \quad \sum_{l=1}^{n} \beta_l^2 = 1, \quad \sum_{l=1}^{n} \alpha_l \beta_l = 0 \quad (32) \\
\sum_{l=1}^{n} \epsilon_l^2 &= 1, \quad \sum_{l=1}^{n} \nu_l^2 = 1, \quad \sum_{l=1}^{n} \epsilon_l \nu_l = 0 \quad (33) \\
\sum_{l=1}^{n} \epsilon_l \alpha_l &= \sqrt{\frac{2\gamma}{\pi(1 - e^{-2\gamma r})}} \left[ \gamma(1 - e^{-\gamma r} \cos(\omega r)) + \omega e^{-\gamma r} \sin(\omega r) \right] \equiv C_1 \quad (34) \\
\sum_{l=1}^{n} \epsilon_l \beta_l &= \sqrt{\frac{2\gamma}{\pi(1 - e^{-2\gamma r})}} \left[ \omega(1 - e^{-\gamma r} \cos(\omega r)) - \gamma e^{-\gamma r} \sin(\omega r) \right] \equiv C_2 \quad (35) \\
\sum_{l=1}^{n} \nu_l \alpha_l &= -\sum_{l=1}^{n} \epsilon_l \beta_l = -C_2, \quad \sum_{l=1}^{n} \nu_l \beta_l = \sum_{l=1}^{n} \epsilon_l \alpha_l = C_1 \quad (36)
\end{align*}
\]

where \(R = \sqrt{(1 - C_1^2 - C_2^2)}\) and \(\theta\) is a free parameter.

B. Solution 2

Another choice for \(\vec{\alpha}\) and \(\vec{\beta}\) is

\[
\begin{align*}
\alpha_1 &= \alpha_2 = \alpha_3 = \alpha_4 = \frac{1}{2} \quad (41) \\
\beta_1 &= -\beta_2 = -\beta_3 = \beta_4 = \frac{1}{2} \quad (42)
\end{align*}
\]

We then obtained \(\vec{\epsilon}\) and \(\vec{\nu}\) to be

\[
\begin{align*}
\epsilon_1 &= D_1 + D_3 \cos(\theta), \quad \epsilon_2 = D_2 + D_3 \sin(\theta), \quad (43) \\
\epsilon_3 &= D_2 - D_3 \sin(\theta), \quad \epsilon_4 = D_1 - D_3 \cos(\theta) \quad (44) \\
\nu_1 &= D_2 + D_3 \sin(\theta), \quad \nu_2 = -D_1 - D_3 \cos(\theta) \quad (45) \\
\nu_3 &= -D_1 + D_3 \cos(\theta), \quad \nu_4 = D_2 + D_3 \sin(\theta), \quad (46)
\end{align*}
\]

where \(D_1 = (C_1 + C_2)/2, \ D_2 = (C_1 - C_2)/2, \ D_3 = \sqrt{1 - (C_1^2 + C_2^2)/2}\) and \(\theta\) is a free parameter which was set to be \(\pi/4\) in our simulations.

Any set of vectors \(\vec{\alpha}', \vec{\beta}', \vec{e}'\) and \(\vec{\nu}'\) obtained by simultaneously rotating \((\text{SO}(4))\) a given set of vectors \(\vec{\alpha}, \vec{\beta}, \vec{e}, \vec{\nu}\) can be used instead of \(\vec{\alpha}, \vec{\beta}, \vec{e}, \vec{\nu}\) itself. This concludes the solution.
\( \vec{\alpha}, \vec{\beta}, \vec{\epsilon} \) and \( \vec{\nu} \) will also be a valid solution of the equations \( \ref{52} - \ref{56} \). It remains to be seen if a particular choice of these vectors is better than others for numerical simulations with finite number of realizations or not.

III. CONCLUSIONS

The Langevin equation for diffusion of charged particles in presence of an external magnetic field is solved exactly. A scheme for sampling the position and velocity is given which is valid for arbitrary values of the friction coefficient of the medium, the strength of the magnetic field and the time step of evolution. The components of the position and velocity are represented as linear combinations of four independent and identically distributed Gaussian random variates. A six parameter family of solutions is obtained for the expansion coefficients. Further studies are required to see if a particular choice of the expansion coefficients is better than all the other possibilities.

IV. APPENDIX

Consider four unimodular vectors \( \vec{\alpha}, \vec{\beta}, \vec{\epsilon}, \vec{\nu} \) satisfying the conditions

\[
\begin{align*}
\vec{\alpha} \cdot \vec{\alpha} &= 1, \quad \vec{\beta} \cdot \vec{\beta} = 1, \quad \vec{\alpha} \cdot \vec{\beta} &= 0 \\
\vec{\epsilon} \cdot \vec{\epsilon} &= 1, \quad \vec{\nu} \cdot \vec{\nu} = 1, \quad \vec{\epsilon} \cdot \vec{\nu} &= 0 \\
\vec{\epsilon} \cdot \vec{\alpha} &= C_1, \quad \vec{\epsilon} \cdot \vec{\beta} = C_2 \\
\vec{\nu} \cdot \vec{\alpha} &= -C_2, \quad \vec{\nu} \cdot \vec{\beta} = C_1
\end{align*}
\]

\( \ref{47} - \ref{50} \)

A. 2-dimensional case

Let us first consider the 2-dimensional case. Here, the most general pair of vectors \( \vec{\alpha} \) and \( \vec{\beta} \) satisfying eq. \( \ref{47} \) can be easily constructed as follows

\[
\vec{\alpha} = (\cos \theta_1, \sin \theta_1), \quad \vec{\beta} = (-\sin \theta_1, \cos \theta_1).
\]

where \( \theta_1 \) is an arbitrary parameter. Since \( \vec{\alpha} \) and \( \vec{\beta} \) are orthonormal, they form a basis in 2-dimensions and hence any other vector can be expressed as linear combinations of these vectors. Therefore \( \vec{\epsilon} \) and \( \vec{\nu} \) can be written as

\[
\begin{align*}
\vec{\epsilon} &= a_1 \vec{\alpha} + a_2 \vec{\beta} \\
\vec{\nu} &= b_1 \vec{\alpha} + b_3 \vec{\beta}
\end{align*}
\]

B. 3-dimensional case

The most general vector \( \vec{\alpha} \) can be written down as

\[
\vec{\alpha} = (\sin \theta_1 \cos \phi_1, \sin \theta_1 \sin \phi_1, \cos \theta_1)
\]

where \( \theta_1 \) and \( \phi_1 \) are arbitrary parameters. The most general vector \( \vec{\beta} \) perpendicular to \( \vec{\alpha} \) is given by

\[
\vec{\beta} = \cos(\zeta)\vec{\beta} + \sin(\zeta)(\vec{\alpha} \times \vec{\eta})
\]

with

\[
\vec{\eta} = (\cos \theta_1 \cos \phi_1, \cos \theta_1 \sin \phi_1, -\sin \theta_1).
\]

and \( \zeta \) is a free parameter. It is obvious that the vectors \( \vec{\alpha}, \vec{\beta}, \vec{\alpha} \times \vec{\beta} \) form a basis in three dimensional space. Then \( \vec{\epsilon} \) can be defined as

\[
\vec{\epsilon} = a_1 \vec{\alpha} + a_2 \vec{\beta} + a_3 \vec{\alpha} \times \vec{\beta}
\]

Using eqs. \( \ref{49} \) and then \( \ref{50} \) we get

\[
\vec{\epsilon} = C_1 \vec{\alpha} + C_2 \vec{\beta} + a_3 \vec{\alpha} \times \vec{\beta}
\]

with \( C_1^2 + C_2^2 + a_3^2 = 1. \) Similar analysis gives

\[
\vec{\nu} = -C_2 \vec{\alpha} + C_1 \vec{\beta} + b_3 \vec{\alpha} \times \vec{\beta}
\]
with $C_1^2 + C_2^2 + b_3^2 = 1$. Substituting for $\vec{e}$ and $\vec{v}$, we get

$$\vec{e} \cdot \vec{v} = -C_1 C_2 + C_1 C_2 + a_3 b_3 = a_3 b_3$$

(61)

which is not zero in general. Hence it is impossible to obtain the four vectors $\vec{\alpha}$, $\vec{\beta}$, $\vec{e}$ and $\vec{v}$ satisfying the constraints eqs. in three dimensions as well. It is, however, possible to obtain solutions in four dimensions, as explicitly demonstrated in the text.