

Dear Editor,

we would like to resubmit for publication to SciPost our manuscript  
<http://arxiv.org/abs/1705.08083v2>.

We thank the referee for her/his helpful comments and remarks, and have modified the manuscript following her/his suggestions. We provide below a point-to-point response to all remarks.

Should the referee find it useful, a pdf version of our manuscript with all changes highlighted in red is available at [https://www.dropbox.com/s/nrf1f7drtw15il5/sci\\_post\\_2017.pdf?dl=0](https://www.dropbox.com/s/nrf1f7drtw15il5/sci_post_2017.pdf?dl=0).

Your sincerely,  
Antonio Piscitelli and Massimo Pica Ciamarra

## Strength

The paper presents a reasonably clear and complete analysis of the motion of a particle in a periodic potential according to a model proposed over 50 years ago by Il'in and Khasminskii.

## Weakness

The model used in the paper is not defined properly. This is especially important since the original paper introducing this model is over 50 years old and may not be easily accessible to all interested researchers. Specifically, in the Il'in-Khasminskii model “instantaneous interaction with the heat bath occurs at a constant rate  $t_c^{-1}$ ”. Does it mean that the interaction events are equally spaced in time? Or, are they distributed according to a probability distribution? Also, for more mathematically minded readers it would be nice to have an equation of motion for the probability distribution within the Il'in-Khasminskii model.

**Reply:** Following this suggestion, in the revised manuscript (Sec. 2) we properly define the model, and discuss the equation of motion of the probability distribution. We also clarify these points below.

In the Il'in-Khasminskii model the time interval between two successive collisions is distributed like  $P(\Delta t) = e^{-\frac{\Delta t}{t_c}}/t_c$  where  $t_c$  is a parameter of the model. In other papers (see e.g. E. Barkai and V. Fleurov, Phys. Rev, E 52 (1995) 137) the case of collision events equispaced in time is also treated. We have clarified this point in Sec.2.

If  $M$  is the mass of the test particle and  $m$  the mass of the bath particle, the reduced masses can be defined as  $\mu_1 = \frac{M-m}{M+m}$  and  $\mu_2 = \frac{2M}{M+m}$ . If  $x$  and  $p$  are the position and the momentum of the test particle in 1-dim,  $F(x) = -\frac{\partial V(x)}{\partial x}$  is the force on the test particle due to the potential and  $u(x, p, t)$  is the probability distribution of finding the particle around  $x$  with momentum around  $p$ , the integro-differential equation that Il'in and Kashminskii found for  $u$  is:

$$\frac{\partial u(x, p, t)}{\partial t} = -\frac{p}{M} \frac{\partial u(x, p, t)}{\partial x} - F(x) \frac{\partial u(x, p, t)}{\partial p} - \frac{1}{t_c} \int_{-\infty}^{\infty} dp' P(p') \left[ u(x, p, t) - u(x, \frac{p - \mu_2 p'}{\mu_1}, t) \right].$$

This equation can be specialized to the case  $M = m$ , that is the case of our paper, as follows:

$$\frac{\partial u(x, p, t)}{\partial t} = -\frac{p}{m} \frac{\partial u(x, p, t)}{\partial x} - F(x) \frac{\partial u(x, p, t)}{\partial p} - \frac{1}{t_c} u(x, p, t) + \frac{1}{t_c \sqrt{2\pi m T}} e^{-\frac{p^2}{2mT}} \bar{u}(x, t)$$

where  $\bar{u}(x, t)$  is the marginal distribution of the position of the particle. In the revised version of the manuscript, we introduce this equation of motion when reviewing previous results. This turns out to be useful, as it allows us to better clarify that we have not tackled the problem solving this complex equation, but rather introducing a complimentary and physically motivated approach based on the notion of ‘flights’.

The standard model to describe stochastic motion (the Brownian motion model) can be derived from a more fundamental (more complete) description of the particle+bath system. While the derivation is approximate, it provides some physical understanding of the assumptions behind this model. It is not clear whether (and how) the Il'in-Khasminskii model follows from the description of the particle+bath system in terms of the coordinates, positions and interaction of the particle and the particles constituting the bath.

**Reply:** To our knowledge there is no formal derivation of the Il'in-Khasminskii model seen as the projection of the motion of the system on the test particle coordinates. In fact the exponential distribution of the time between collisions is a simplifying assumption. It may not exactly correspond to the actual distribution in most specific physical cases like hard-spheres (see P. Visco, F. van Wijland, E. Trizac, Phys. Rev. E 77, 041117 (2008)), but it has the clear physical meaning

that the process of interaction with the heat bath is assumed to be Markovian, which is approximately true in many circumstances.

The Il'in-Khasminskii model can be seen as a possible generalization of the Brownian motion, useful when the assumptions of the Brownian Motion are not realized. The Brownian Motion has been rigorously retrieved by Il'in and Khasminskii themselves from their model when  $t_c \rightarrow 0$  and  $M \gg m$ . This limit is sometimes addressed as the diffusion approximation. It is valid when the time between collisions is much shorter than all the other relevant timescales and hence can be neglected. This condition is not always realized. For instance, it is not realized in systems undergoing strong and rare fluctuations, like a real gas at low pressure. Indeed, the Il'in-Khasminskii model has been used for the calculation of the reaction rates in such gases, where the potential was intended along the reaction coordinate.

In Sec. 2, after Eqs. 2 and 3, we added a sentence addressing this point.

The physical interpretation and thus the estimation of the parameters in the Langevin equation describing the standard model is reasonably clear. How could one estimate  $t_c$ , i.e. the characteristic time of the Il'in-Khasminskii model?

**Reply:** The time  $t_c$  is the time of correlation of the position and momentum. We stress however that in the Brownian Motion case, where  $M \gg m$ , the correlation in time is due to the inertia of the test particle. In the case of “strong collision”, that is  $M = m$ , the time correlation should be thought of as the time of the mean free path of the molecules. It can thus be related to the inverse of the pressure of the gas.

In the same paragraph in Sec. 2 where we address the second point, we also clarify the physical meaning of  $t_c$ .

The paper introduces and uses a variety of acronyms. Some of them are relatively non-standard (e.g. VhD). This makes the paper a bit difficult to follow.

**Reply:** We eliminated the acronym VhD for Van Hove, substituting with the explicit expression, and reduced the number of acronyms to improve clarity.

Some figures (e.g. panels (d-f) of Fig. 7) are difficult to read. The inset in panel c of Fig. 7 is impossible to read in the standard size.

**Reply:** The inset shows the MSD as a function of  $\Gamma_\tau \Delta t$  for comparison with panel (f). Since it is well clarified in the text that we see

non gaussian Van Hove distributions at times at which we see diffusive MSD, we decided to eliminate the panel. We have also modified panels (d-f) of Fig. 7 to improve their readability.

## Report

This paper discusses the application of an approach introduced by Il'in and Khasminskii to the motion of a stochastic particle in a periodic potential. It provides additional details regarding previously described results. It discusses the transition from overdamped to underdamped motion. It shows that according to the Il'in-Khasminskii model, diffusive mean-squared displacement can coexist with non-Gaussian probability distribution of displacements. I recommend that the paper is accepted after the authors considered the (relatively minor) changes requested below.

**Reply:** We thank the reviewer for his/her supportive statement.

## Requested changes

I would appreciate some suggestions regarding the applicability of the present model and, in particular, how "the loss of a typical time ... length scale" could be accessed from the analysis of the trajectories. For example, if one had a trajectory, how would one decide whether to describe it using the present model or the Brownian motion model?

**Reply:** We thank the reviewer for his/her supportive statement.

The trajectories of the Brownian model and of the present model have an important difference. The trajectory of a Brownian particle is selfsimilar and nowhere differentiable. Conversely, in the present model trajectories are differentiable (which is what allows for the definition of flight). This difference emerges when the trajectories are observed with a temporal resolution better than  $t_c$  is needed. On a timescale larger than  $t_c$  the trajectories are indistinguishable (see Fig.1 of A. Piscitelli, M.P. Ciamarra Scientific Reports 7, 41442 (2017)).

The time resolution, because of the selfsimilarity, translates in a spatial resolution. In particular, considering two systems, one of Il'in Khasminskii type with collision time  $t_c$  and one Brownian with viscous coefficient  $\gamma = t_c^{-1}$ , in the overdamped case ( $t_c \ll \omega_b^{-1}$ ) the length resolution around the maximum of the potential sufficient to determine the type of model, according to the trajectory appearing respectively differentiable or not differentiable, is of order  $t_c\sqrt{T/m}$ .

The trajectories of the model are such that for  $t_c < 1/\sqrt{2}$  the flights crossing the maximum of the potential have the typical size mentioned above and a duration proportional to  $t_c$ , while for  $t_c > 1/\sqrt{2}$  these

typical scales are lost. In the underdamped limit the two models markedly differ.

Another difference between the two models is observed in the number of wells traversed in a time  $t_c$  ( $\gamma^{-1}$ , that a low temperature is much larger for the Il'in Kashminskii dynamics).

We added a comment about this point at the end of Sec.4.

The model used in the paper should be properly defined.

**Reply:** We have added a paragraph to Sec. 2 where we properly define the considered model.

The number of acronyms used should be reduced.

**Reply:** We eliminated the acronym VhD for Van Hove distribution and BnG for Brownian non-Gaussian, substituting with the explicit expression.

Readability of the figures should be improved.

**Reply:** We have eliminated the inset of Fig. 7c. We increased the size of the labels in figure 7 panels d, e and f and eliminated the Brownian Motion curves in panels a, b, d and e, mentioning in the text that they are indistinguishable from the Il'in Kashminskii ones.

## Minor points

The authors write in the Abstract that they "introduce a physically motivated theoretical approach". Rather, they use a previously introduced approach (by Il'in and Khasminskii) to describe motion in a periodic potential.

**Reply:** We modified the mentioned sentence into: "We analyze the classical problem of the stochastic dynamics of a particle confined in a periodic potential, through the so called Il'in and Khasminskii model, with a novel semi-analytical approach". Indeed while the model we are describing is in fact the Il'in and Khasminskii model, some of the conclusions that we draw couldn't have been obtained from the Il'in and Khasminskii integro-differential equation, that is considerably difficult. The notion we start from for an approximated analytical treatment, the flight, has a clear physical interpretation with no immediate counterpart in the Brownian Motion. This approach could be considered as complementary to the usual Fokker-Planck type approach for this particular problem.

We also added a sentence at the very beginning of Sec.IIIb clarifying this point.

According to the caption, the full line in Fig. 2a is an empirical fit rather than a prediction and thus should be labeled as such.

**Reply:** We have dashed the mentioned line and properly labeled it.

On p.7 the authors attribute the plateau to "the interaction with the thermal noise and confining barrier". I think the noise itself does not cause the plateau?

**Reply:** We agree with the referee. We modified the sentence into: "The MSD displays a ballistic regime, followed by a plateau due to the confining potential. Unlike in both the over and under damped regime the time of the beginning of the plateau coincides with the end of the ballistic regime due to the interaction with the heat bath."

Some more editing (e.g. removing "Langeving" on p. 1) should be done.

**Reply:** We corrected the typo.

## Notes

We fixed a typo in the formula in the paragraph following Eq. 1. We added Eq. 19, while the old Eq. 18 becomes Eq. 20. Unlike stated before, Eq. 19, rather than Eq. 20, holds at all the temperatures; Eq. 20 only holds at low temperature.