Truncated Lévy Flights and Weak Ergodicity Breaking in the Hamiltonian Mean Field Model

A. Figueiredo, T. M. Rocha Filho, and M. A. Amato
Instituto de Física and International Center for Condensed Matter Physics
Universidade de Brasília, CP: 04455, 70919-970 - Brasília, Brazil

Z. T. Oliveira Jr
Departamento de Ciências Exatas e Tecnológicas,
Universidade Estadual de Santa Cruz,
CEP 45662-900 - Brazil and
International Center for Condensed Matter Physics
Universidade de Brasília, CP: 04455, 70919-970 - Brasília, Brazil

R. Matsushita
Departamento de Estatística
Universidade de Brasília, CP: 04455,
70919-970 - Brasília, Brazil

Abstract

The dynamics of the Hamiltonian mean field model is studied in the context of continuous time random walks. We show that the sojourn times in cells in the momentum space are well described by a Lévy truncated distribution. Consequently the system in weakly non-ergodic for long times that diverge with the number of particles. For a finite number of particles ergodicity is only attained for very long times both at thermodynamical equilibrium and at quasi-stationary out of equilibrium states.

PACS numbers: 05.20.-y, 05.20.Dd, 05.10.Gg
Ergodicity is an important concept in statistical mechanics [1, 2] and essentially states that ensemble averages are equal to the time average over a single trajectory of the system or that the sojourn time on a given region is proportional to its ensemble measure. For particles in an external potential, ergodicity implies that time averages over a single particle trajectory is equal to the average over many particles at a fixed time. The latter case has recently been observed experimentally for the diffusion of molecules on a nanostructured porous glass [3]. Strong ergodicity breaking occurs if some region of the phase space is not accessible by the system trajectory. On the other hand weak non-ergodic behavior corresponds to a situation where every state can be reached but the occupation statistics is not equal to the ensemble measure [4]. The statistical mechanics of weakly non-ergodic systems in the context of continuous time random walk (CTRW) was addressed by Rebenishek and Barkai [5]. In this approach the system can be in $M$ different states, such that a given observable $O$ admits the respective $M$ values $O_k$ for $k = 1, \ldots, M$. The time average of this observable is then

$$
\mathcal{O} = \frac{1}{t_{\text{tot}}} \sum_{k=1}^{M} t_k O_k, \quad t_{\text{tot}} = \sum_{i=k}^{i} t_k,
$$

where $t_k$ is the residence time, i.e. the total time spent by the system in state $k$ and $t_{\text{tot}}$ the total observation time. The sojourn time $t_{k,j}^{(s)}$ is the time spent in state $k$ during the $j$-th visitation, and therefore $t_k = \sum_j t_{k,j}^{(s)}$. Supposing that the sojourn times are independent identically distributed (iid) variables and owing to Lévy generalized central limit theorem, the probability distribution of residence time $t_k$ can be described by a one-sided Lévy distribution $f_k^{(\alpha)}(t)$ with Laplace transform [5, 6]:

$$
\int_{0}^{\infty} f_k^{(\alpha)}(t) e^{-st} dt = e^{-\gamma_k s^{\alpha/2}},
$$

for $0 < \alpha \leq 2$, $\alpha = 2$ corresponding to the Gaussian distribution, and $\gamma_k$ is a constant factor. The exponent in the right-hand side of eq. (2) was chosen to coincide with the exponent in the characteristic function of the Lévy distribution [6]. An important feature is that the moments $<|t|^\mu>$ of the Lévy distribution diverge for $\mu > \alpha$. The distribution of the possible different values of the time averages $\mathcal{O}$ is given by [6]:

$$
F^{(\alpha)}(\mathcal{O}) = -\frac{1}{\pi} \lim_{\epsilon \to 0} \text{Im} \sum_{k=1}^{M} \frac{\gamma_k (\mathcal{O} - O_k + i\epsilon)^{\alpha/2-1}}{\sum_{k=1}^{M} \gamma_k (\mathcal{O} - O_k + i\epsilon)^{\alpha/2}}.
$$

In the limit $\alpha \to 2$ eq. (3) reduces to $F^{(2)}(t) = \delta(\mathcal{O} - \langle \mathcal{O} \rangle)$, where $\langle \mathcal{O} \rangle = \sum_k \gamma_k O_k$, and the coefficients $\gamma_k$ are equilibrium (stationary) probabilities. As a consequence ensemble
and time averages are equal and the system is ergodic. The case of non iid sojourn times
statistics have been addressed in Ref. [7].

In the present work we discuss a system with sojourn time statistics satisfying a truncated
Lévy flight defined as [8]:

\[
\tilde{f}(\alpha)(t) = \begin{cases} 
  cf^{(\alpha)}(t), & \text{if } |t| < L, \\
  0, & \text{otherwise}, 
\end{cases}
\] (4)

where \( c \) is a normalization constant and \( L > 0 \). Instead of an abrupt truncation at \( t = L \) it
is also possible to use a smooth truncation with a function decaying faster than a power law.
Such functions have finite moments, and therefore the sum of random variables drawn from it
converge to a Gaussian distribution. Nevertheless this convergence is extremely slow and for
a finite sum \( X^{(n)} = \sum_{k=1}^{n} t_k \), with \( t_k \) drawn from the distribution in eq. (4), the distribution
remains close to a true stable Lévy distribution sometimes for large \( n \), displaying a typical
scaling behavior before a crossover to a Gaussian behavior. The probability density for \( X^{(n)} \)
being zero is given for small \( n \) by [8]:

\[
P^{(n)}(0) = \frac{\Gamma(1/\alpha)}{\pi \alpha (\gamma n)^{1/\alpha}},
\] (5)

with \( \gamma \) a scale factor and for large \( n \) we have a Gaussian distribution:

\[
P^{(n)}(0) = \left[ \sigma \sqrt{2\pi n^{1/2}} \right]^{-1},
\] (6)

where \( \sigma \) is the standard deviation. The crossover value of \( n \) from a pure Lévy to the Gaussian
behavior predicted by the central limit theorem increases with \( L \). The statistics of sojourn
times is a one-sided Lévy distribution, but this analysis can be performed by symmetrizing
the distribution as \( f^{(\alpha)}_{k}(-t) = f^{(\alpha)}_{k}(t) \). The distributions obtained from this sum all collapse
in the same function under the scaling:

\[
X \rightarrow n^{-1/\alpha} X \text{ and } P^{(n)}(X) \rightarrow n^{1/\alpha} P^{(n)}(X).
\] (7)

Examples of weakly non-ergodic systems include laser cooling of trapped atoms [9], dif-
fusion of lipid granules in living cells [10], blinking quantum dots [11, 12] and glass dy-
namics [4]. In the present letter we study the ergodic properties of a classical Hamiltonian
system with a long-range interaction considered as a CTRW as a preliminary step of a more
thorough investigation of more general classes of long-range interacting systems, that have
drawn some attention in the last two decades [13–16], and can have some unusual properties such as anomalous diffusion, aging, negative heat capacity at equilibrium, non-Gaussian quasi-stationary states and a relaxation time to equilibrium diverging with the number \( N \) of particles. They are characterized by a pair-interaction potential decaying asymptotically as \( r^{-a} \), \( a < D \) with \( D \) the spatial dimensions [17]. Some important physical systems in this category are self-gravitating systems and non-neutral plasmas (see [14] for more examples). Despite their interest their dynamics is not completely understood due to inherent difficulties and a few toy models were introduced in the literature in order to simplify the understanding of their intricate behavior. Among them we cite the Hamiltonian mean field (HMF) model [18], which has become a sort of ground test for many numerical and analytical studies, and defined by the Hamiltonian:

\[
H(p, \theta) = \frac{1}{2} \sum_{i=1}^{N} p_i^2 + \frac{1}{2N} \sum_{i,j=1}^{N} \left[ 1 - \cos(\theta_i - \theta_j) \right].
\]  

(8)

This system can be interpreted as consisting of \( N \) classical rotors globally coupled and with unit moment of inertia and its thermodynamical equilibrium properties can be determined analytically [18, 19]. It has a second order phase transition from a spatially homogeneous to an inhomogeneous phase, a rich structure of non-equilibrium phase transitions [20] and the great advantage that molecular dynamics simulations scales with the number \( N \) of particles instead to the usual \( N^2 \) scaling allowing simulations with a large number of particles.

For classical Hamiltonian systems with long-range interactions in the limit \( N \to \infty \) the one-particle distribution function exactly satisfies the mean field Vlasov equation [22]. Thence we only have to consider the dynamics of a single particle evolving in the mean field of the remaining particles. Quasi-stationary states thus correspond to the infinite number of stable stationary states of the Vlasov equation. For finite \( N \) small collisional corrections must be considered resulting in a secular evolution of the quasi-stationary states.

The ergodic behavior of the HMF model has been previously discussed by some of the authors in Ref. [21] showing that the time average of the velocity of a single particle is equal to the ensemble average over the \( N \) particles only after a very long time of the order of the relaxation of the system to true thermodynamical equilibrium. Here we discuss this behavior in the framework of the CTRW in the momentum space by performing molecular dynamics simulations for the Hamiltonian in eq. (8). The momentum space is divided in cells of width \( \Delta p \), and each cell is then taken as a different discrete state. We consider
here two types of statistically stationary states: thermodynamical equilibrium and a stable non-Gaussian (quasi) stationary state with a waterbag one-particle momentum distribution $\rho(p) = 1/2p_0$ if $-p_0 < p < p_0$ and zero otherwise. We consider at this point spatially homogeneous distributions resulting in a vanishing force in the mean-field limit but with small fluctuations due to collisional corrections for finite $N$ which cause small cumulative changes in the momenta. The temperature for the equilibrium case is chosen as $T = 0.8$ and for the non-equilibrium case we chose $p_0 \approx 2.68$ which yields an total energy per particle $e = 0.8$. We start by considering the statistics of sojourn times for different cells of width $\Delta p = 0.4$ shown in Fig. 1 for the equilibrium case and $N = 100,000$ particles. The distributions obtained are equal up to the noise level, and by supposing that they are also independent we have an iid process. The time evolution of the velocity of a single particle is shown in the left panel of Fig. 2 for $N = 500,000$ particles such that the fluctuations of the field are already quite small illustrating clearly the trapping of the velocity in regions of the momentum space with rapid movements between different traps. The corresponding sojourn times for all cells with width $\Delta = 0.4$ are shown in the right panel of Fig. 2. The right panel of Fig. 2 show the sojourn times in cells of width $\Delta p = 0.4$. As the statistics of sojourn times are the same the sojourn times are taken from all cells which allows a better statistical accuracy in our analysis.

In order to show that the sojourn time statistics satisfy a truncated Lévy distribution we perform a sum of $n$ sojourn times randomly chosen among those obtained from our
FIG. 2. Left Panel: Velocity of a particle as a function of time for \( N = 500,000 \) and total simulation time \( t_f = 10^7 \) for the Gaussian distribution. Right panel: Corresponding sojourn times.

FIG. 3. Left Panel: Probability density \( P^{(n)}_N(0) \) as a function of the number of summed variables for different values of the number \( N \) of particles and normalized with respect to the probability at zero of the original distribution \( (n = 1) \) for the equilibrium state. The straight line is the curve obtained from a fitting for the initial part of the curve for \( N = 200,00 \) with \( \alpha = 0.603 \). Right Panel: The same as the left panel but for the water-bag state, the straight line corresponds to \( \alpha = 0.51 \). In both panels all curves tend to a \( t^2 \) power law with increasing \( n \).

simulations and also randomly choosing its sign (this is equivalent to symmetrizing the distribution). The left panel of Figure 3 shows the probability at zero \( P^{(n)}(0) \) as a function of \( n \), where the crossover from the scalings in eq. (5) to eq. (6) is clearly visible. The right panel shows the same probability for the non-equilibrium stationary waterbag state. The value of the coefficient \( \alpha \) in the truncated Lévy distribution in eqs. (2,4) can be determined from the sojourn times using maximum likelihood method [23, 24] and are shown in table I.
for different number of particles. They are obtained by considering the distribution $f^{(n)}(T)$ as a true (non-truncated) Lévy distribution, which is reasonable if $L$ is large enough, but can introduce some errors in the estimation of the exponent $\alpha$. This explains the difference between the values of $\alpha$ obtained by this method and those determined using a fitting procedure as described in the caption of Fig. 3.

The second moments, $<t^2> = (1/S) \sum_{k=1}^{S} t^2_k$ of the distribution of sojourn times, where $S$ is the number of sojourn times, are shown for different values of $N$ in figure 4 such that a power law increase with $N$ is evident, which shows that the effective truncation value $L$ diverges with $N$. Figure 5 shows the tail of the distribution for $N = 50,000$ with the straight line corresponding to a power law $t^{-(1+\alpha)}$ with $\alpha$ given in table I. Figure 6 shows the symmetrized distribution functions of sojourn times for a few values of $n$ (left panel) and the collapsed distribution obtained from the scaling in eq. (7) (right panel), showing a good agreement as expected for a Lévy distribution.

From our results we can assert that the HMF model becomes ergodic only after a very long time such that the sum of sojourn times obeying a truncated Lévy distribution converge very slowly to a Gaussian distribution. This sum yields the distribution of residence times which at it turn determine the ergodic properties of the system. This time corresponds to the crossover between Lévy and Gaussian behaviors in the graphics in Figure 3 and for shorter times, which are effectively still very long, the system is weakly non-ergodic. Our results also show that this crossover time diverges with the number of particles in the system. This is the first time, up to the authors knowledge, that non-ergodic behavior in a system with

| $N$         | $\alpha_{eq}$ | $\alpha_{wb}$ |
|-------------|---------------|---------------|
| 10,000      | 0.6730        | 0.9993        |
| 50,000      | 0.5849        | 0.6868        |
| 100,000     | 0.5648        | 0.6451        |
| 200,000     | 0.5528        | 0.6129        |
| 500,000     | 0.5596        | 0.6265        |

TABLE I. Values of $\alpha$ in eq. (2) for the thermodynamical equilibrium ($\alpha_{eq}$) and waterbag distribution ($\alpha_{wb}$).
FIG. 4. Moments of the second moment $\langle t^2 \rangle$ for the equilibrium and waterbag distributions.

FIG. 5. Log-Log plot of the tail of the distribution function of sojourn times $t_s$ for the equilibrium case for $N = 50,000$. The straight is a power law $t^{-(1+\alpha)}$ with $\alpha = 0.5849$.

long-range interactions is shown to be related to Lévy flights in momentum space. We also performed a similar study for non-homogeneous states with similar results. A more thorough analysis for the HMF model and other models with long-range interactions is under course and will be the subject of a future publication.

The authors would like to thank CNPq and CAPES (Brazilian government agencies) for partial financial support. A. F. and T. M. R. F. would like to thank R. Venegeroles for many useful discussions.

[1] G. D. Birkhoff, PNAS 17, 656 (1931).
FIG. 6. Left panel: distribution for the sum $X^{(n)}$ of random variables for $n = 0, 2, 4, 6, 8, 10$ for the Gaussian equilibrium case, where higher values of $n$ has a smaller probability for zero. Right panel: collapse of the distribution functions by the scaling in eq. (7) with $\alpha = 0.5596$ as the best estimate in table I.

[2] A. I. Kinchin, *Mathematical Foundations of Statistical Mechanics*, (Dover, New York, 1949).
[3] F. Feil, S. Naumov, J. Michaelis, R. Valiullin, D. Enke, J. Kärger and C. Bräuchle, Angew. Chem. Int. Ed. **51**, 1152 (2012).
[4] J. P. Bouchaud, J. Phys. I France **2**, 1705 (1992).
[5] A. Rebenshtok and E. Barkai, J. Stat. Phys. **133**, 565 (2008).
[6] G. Samorodnitsky and M. S. Taqqu, *Stable Non-Gaussian Random Processes* (Chapman & Hall/CRC, London, 2000).
[7] A. Saa and R. Venegeroles, Phys. Rev. E **82**, 031110 (2010).
[8] R. N. Mategna and H. E. Stanley, Phys. Rev. Lett. **73**, 2946 (1994).
[9] B. Saubamea, M. Leduc and C. Cohen-Tanoudji, Phys. Rev. Lett. **83**, 3796 (1999); Leduc and C. Cohen-Tanoudji, Phys. Rev. Lett. **83**, 3796 (1999).
[10] J.-H. Jeon, V. Tejedor, S. Burov, E. Barkai and C. Selhuber-Unkel, Phys. Rev. Lett. **106**, 048103 (2011).
[11] X. Brokmann, J.-P. Hermier, G. Messin, P. Desbiolles, J.-P. Bouchaud and M. Dahan, Phys. Rev. Lett. **90**, 120601 (2003).
[12] G. Margolin and E. Barkai, Phys. Rev. Lett. **94**, 080601 (2005).
[13] A. Campa, T. Dauxois and S. Ruffo, Phys. Rep. **480**, 57 (2009).
S. Ruffo, E. Arimondo and M. Wilkens Eds. (Springer, Berlin, 2002).

[15] Dynamics and Thermodynamics of Systems with Long-Range Interactions: Theory and Experiments, A. Campa, A. Giansanti, G. Morigi and F. S. Labini (Eds.), AIP Conf. Proceedings Vol. 970 (2008).

[16] Long-Range Interacting Systems, Les Houches 2008, Session XC, T. Dauxois, S. Ruffo and L. F. Cugliandolo Eds. (Oxford Univ. Press, Oxford, 2010).

[17] T. Dauxois, S. Ruffo, E. Arimodo and M. Wilkens, Dynamics and Thermodynamics of Systems with Long-Range Interactions: An Introduction, in [14].

[18] M. Antoni and S. Ruffo, Phys. Rev. E 52, 2361 (1995).

[19] T. M. Rocha Filho, M. A. Amato and A. Figueiredo, J. Phys. A 42, 165001 (2009).

[20] T. M. Rocha Filho, M. A. Amato, and A. Figueiredo, Phys. Rev. E 85, 062103 (2012).

[21] A. Figueiredo, T. M. Rocha Filho and M. A. Amato, Europhys. Lett. 83, 30011 (2008).

[22] W. Braun and K. Hepp, Commun. Math. Phys. 56 (1977) 101.

[23] A. Feuerverger and P. McDunnough, J. Am. Stat. Assoc. 76, 379-387 (1981).

[24] C. R. Rao, Linear statistical inference and its applications, 2nd Ed. (John Wiley & Sons, New York, 2002).