Quasistationary States and the Range of Pair Interactions

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"Quasistationary" states are approximately time independent out of equilibrium states which have been observed in a variety of systems of particles interacting by long-range interactions. We investigate here the conditions of their occurrence for a generic pair interaction $V(r \to \infty) \sim 1/r^\gamma$ with $\gamma > 0$, in $d > 1$ dimensions. We generalize analytic calculations known for gravity in $d = 3$ to determine the scaling parametric dependences of their relaxation rates due to two-body collisions, and report extensive numerical simulations testing their validity. Our results lead to the conclusion that, for $\gamma < d - 1$, the existence of quasistationary states is ensured by the large distance behavior of the interaction alone, while for $\gamma > d - 1$ it is conditioned on the short distance properties of the interaction, requiring the presence of a sufficiently large soft core in the interaction potential.

In recent years there has been renewed interest in the statistical physics of long-range interactions (for a review, see, e.g., [1]), a subject which has been treated otherwise mostly in the astrophysical literature for the specific case of gravity. The defining property of such interactions is the nonadditivity of the potential energy of a uniform system, which corresponds to the nonintegrability at large distances of the associated pair interaction, i.e., a pair interaction $V(r \to \infty) \sim 1/r^\gamma$ with $\gamma < d$ in d space dimensions. The equilibrium thermodynamic analysis of these systems is very different to the canonical one for short-ranged interactions (with $\gamma > d$), leading notably to inhomogeneous equilibria as well as other unusual properties—e.g., nonequivalence of the statistical ensembles, negative specific heat in the micro-canonical ensemble. Studies of simple toy models have shown that, like for gravity in $d = 3$, these equilibria (when defined) are reached only on time scales which are extremely long compared to those characteristic of the mean-field dynamics. On the latter time scales one observes typically the formation, through "violent relaxation," of so-called "quasistationary" states (QSS), interpreted theoretically as stable stationary states of the Vlasov equation (which describes the kinetics in the mean-field limit). In this Letter we consider whether the occurrence of such QSS driven by mean-field dynamics can be considered as a behavior arising generically when there are long-range interactions in play. Using both simple analytical results and numerical simulations, we argue for the conclusion that it is only for $\gamma < d - 1$, i.e., when the pair force is absolutely integrable at large separations, that QSS can be expected to occur independently of the short distance properties of the interaction. For $\gamma >$ $d - 1$, on the other hand, their occurrence will be conditioned strongly also on short distance properties, and thus cannot be considered to be a result simply of the long-range nature of the interaction. Our analysis shows the relevance of a classification of the range of interactions according to the convergence properties of forces rather than potential energies which has been formalized in [2].

We proceed by first generalizing a calculation originally given by Chandrasekhar for Newtonian gravity to a system of N particles interacting by a pair potential $V(r) = \frac{g}{r^\gamma}$ (where g is a coupling constant). This calculation, which numerical studies indicate is accurate both parametrically and quantitatively for gravity (see, e.g., [3–7]), will give us an estimate of Γ_2, the relaxation rate due to two-body collisions (i.e., the inverse of the time scale on which a typical particle's velocity is randomized by such interactions). Denoting by τ_{mf} the characteristic time for the formation of a QSS (i.e., of the mean-field dynamics), the criterion for the existence of QSS we will then study is

$$\Gamma_2 \tau_{\mathrm{mf}} \to 0 \quad \text{when } N \to \infty, \tag{1}$$

where the limit $N \to \infty$ corresponds to the mean-field or Vlasov limit [1]. Indeed, if this condition is not satisfied, it implies that there is no mean-field regime in which QSS may form.

Following the treatment for the case of gravity (see, e.g., [3], Sec. 1.2.1) we consider a test particle of velocity v crossing a system in a QSS, assumed spherical and of radius R and approximated as homogeneous. We estimate first the rate of relaxation due to soft two-body collisions by calculating Δv^2, the mean square velocity change of a

particle per crossing (i.e. in a time of order τ_{mf}) due to such
collisions. It is straightforward to show that

$$\frac{\Delta v^2}{v^2} \sim N\left(\frac{g}{mv^2 R^\gamma}\right)^2 \int_{b_{\min}/R}^{b_{\max}/R} \frac{dx}{x^{2\gamma-d+2}}, \qquad (2)$$

where $b_{\min}$ is the minimal impact parameter at which
the scattering is soft (i.e., the deflection angle is small),
defined by

$$\frac{|g|}{mv^2 b_{\min}^\gamma} \sim 1, \qquad (3)$$

and $b_{\max}$ is the maximal impact parameter for two-body
collisions. In these formulas, and in what follows below,
we use the symbol $\sim$ to indicate that the numerical factors
in all expressions have been dropped, leaving only the
parametric dependences which are relevant to our consid-
erations here. In the case of gravity in $d = 3$ the choice of
$b_{\max}$ has been a source of debate, with numerical simula-
tions indicating that $b_{\max} \sim R$ accounts better for results
than the more evident choice $b_{\max} \sim \ell$, the mean interpar-
ticle separation (see, e.g., [4]). We consider in what follows
both possibilities, and will see that our central results are
not in fact sensitive to which is correct. We have also
implicitly assumed $d > 1$ and $\gamma > 0$.

We now write

$$\Gamma_2 \tau_{\mathrm{mf}} = \Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}} + \Gamma_{\mathrm{hard}} \tau_{\mathrm{mf}}, \qquad (4)$$

where the first contribution is that considered above, and
the second is the remaining one from hard scatterings, i.e.,
collisions with impact factors $b < b_{\min}$. Taking now that
$\tau_{\mathrm{mf}} \sim \frac{R}{v}$, it is straightforward to deduce from Eq. (2) that,
for sufficiently large N,

$$\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}} \sim \begin{cases} N^{-1}\left(\frac{b_{\max}}{R}\right)^{-2\gamma+d-1} & \text{if } \gamma < (d-1)/2, \\ N^{-1}\left(\frac{R}{b_{\min}}\right)^{2\gamma-d+1} & \text{if } \gamma > (d-1)/2, \end{cases} \qquad (5)$$

if $b_{\min}/b_{\max} \ll 1$ for large N. To infer these scalings we
need only (as in the corresponding derivation for the case
of gravity [3]) use the fact that the QSS is, by definition, a
virialized state, i.e., we take

$$\frac{g}{mv^2 R^\gamma} \sim \frac{1}{N}\frac{gN^2}{(mNv^2)R^\gamma} \sim \frac{1}{N}\frac{U}{K} \sim \frac{1}{N}, \qquad (6)$$

where U, the total potential energy of the QSS, and K, its
total kinetic energy, have a fixed ratio because of virializa-
tion. This scaling with N corresponds to that in the usual
mean-field or Vlasov limit, in which U and K both scale in
the same way with N.

Using again the scaling Eq. (6), the definition Eq. (3)
gives

$$b_{\min} \sim RN^{-(1/\gamma)}. \qquad (7)$$

Note first that this implies $b_{\min}/b_{\max} \to 0$ as $N \to \infty$ for
any $\gamma > 0$ if $b_{\max} \sim R$, and for any $0 < \gamma < d$ if $b_{\max} \sim \ell \sim RN^{-1/d}$, so that Eq. (5) is indeed valid in these cases.
Using now again Eq. (7) in Eq. (5) we obtain the scaling

$$\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}} \sim \begin{cases} N^{-(1+|\delta|)} & \text{if } \gamma < (d-1)/2, \\ N^{-(d-1-\gamma)/\gamma} & \text{if } \gamma > (d-1)/2, \end{cases} \qquad (8)$$

where $\delta = 0$ if $b_{\max} \sim R$, and $\delta = (-2\gamma + d - 1)/d$ if
$b_{\max} \sim RN^{-1/d}$. It follows that, for $\gamma > d - 1$, the contri-
bution of soft two-body scatterings alone diverges at large
N, so that the criterion (1) cannot be satisfied in this case
for the "candidate" QSS. For any $\gamma < d - 1$, on the other
hand, the contribution $\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}}$ vanishes as $N \to \infty$. It is
simple to show, in this case, that $\Gamma_{\mathrm{hard}} \tau_{\mathrm{mf}}$ also goes to zero
when $N \to \infty$, and thus that the condition (1) for the
existence of QSS may be satisfied. To do so it is sufficient
to consider that this contribution can be bounded below by
that from an "exactly hard" core with radius $\epsilon = b_{\min}$, i.e.,
$V(r) = \infty$ for $r < b_{\min}$. Estimating the collision rate on
such a core as $\Gamma_{\mathrm{hc}} \sim n\sigma v$ where n is the mean density and
$\sigma \sim \epsilon^{d-1}$ (the cross section), we obtain

$$\Gamma_{\mathrm{hc}} \tau_{\mathrm{mf}} \sim N\left(\frac{\epsilon}{R}\right)^{d-1} \sim N^{-(d-1-\gamma)/\gamma} \qquad (9)$$

when we take $\epsilon = b_{\min}$, with the latter scaling as in Eq. (7).
It follows that $\Gamma_{\mathrm{hard}} \tau_{\mathrm{mf}} \leq \Gamma_{\mathrm{hc}} \tau_{\mathrm{mf}} \to 0$ as $N \to \infty$ for $\gamma < d - 1$. Further it follows from the inferred scaling of
$\Gamma_{\mathrm{hc}} \tau_{\mathrm{mf}}$ that, for $\gamma < d - 1$, the total rate Γ_2 will scale as
calculated for Γ_{soft} in Eq. (8). In other words, an exact
calculation including Γ_{hard} should give, at most, a Γ_2 larger
than Γ_{soft} by a numerical factor.

A corollary of these results, which are summarized in
Table I, is that, for a QSS to exist in the case that $\gamma > d - 1$, the pair potential must include a sufficiently large soft
core. Indeed to remove the divergence of $\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}}$ in this
case, we must introduce a smoothing of the potential at a
scale ϵ which vanishes more slowly than $b_{\min}$ in Eq. (7). In
this case $\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}}$ is given by the second expression in Eq.
(5) but with $b_{\min}$ replaced by ϵ. Keeping ϵ/R constant, for
example, gives $\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}} \sim N^{-1} \to 0$ as $N \to \infty$ for any γ.
If the core is "exactly soft," i.e., $V(r) = g/\epsilon^\gamma$ for $r < \epsilon$ we
have $\Gamma_{\mathrm{hard}} = 0$ and the satisfaction of the condition Eq. (1)
follows. If the core is hard, as envisaged above, it is clear
that the same is not true. Indeed it is simple to check using
Eq. (9) that it is not possible to choose ϵ in order to satisfy
both $\Gamma_{\mathrm{hc}} \tau_{\mathrm{mf}} \to 0$ and $\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}} \to 0$ simultaneously as $N \to \infty$ for $\gamma > d - 1$.

TABLE I.   Summary of two-body collision rates (without core).

$0 < \gamma < \frac{d-1}{2}$	Soft collisions at $\sim b_{\max}$ dominate $\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}} \sim N^{-(1+|\delta|)} \gg \Gamma_{\mathrm{hard}} \tau_{\mathrm{mf}}$
$\frac{d-1}{2} < \gamma < d - 1$	Collisions at $\sim b_{\min}$ dominate $\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}} \sim N^{-(d-1-\gamma/\gamma)} \geq \Gamma_{\mathrm{hard}} \tau_{\mathrm{mf}}$
$\gamma > d - 1$	$\Gamma_{\mathrm{soft}} \tau_{\mathrm{mf}}$ and $\Gamma_{\mathrm{hard}} \tau_{\mathrm{mf}}$ divergent in N

These results lead then to the primary conjecture of this article: for pair potentials with $V(r \to \infty) \sim 1/r^\gamma$, QSS can always exist if there is a sufficiently large soft core, but only for $\gamma < d - 1$ can they exist when such a core is not present (i.e., when its size $\epsilon \to 0$). The validity of this conclusion rests evidently on the assumption that the dominant correction to the mean-field dynamics is, just as for gravity in $d = 3$, two-body collisionality. More specifically we also require the parametric dependences of the inferred relaxation rates, which have been derived using various simplifying approximations (notably that of homogeneity both in configuration and velocity space). We now present results of numerical simulations (in $d = 3$) which test their validity. We focus here on the crucial result above: the parametric dependence of the two-body scattering rate due to soft scatterings in Eq. (5), for the range $\gamma > (d - 1)/2$.

We perform molecular dynamics simulations using a version of the publicly available gravity code GADGET2 [8]. We have modified the force routine in the tree-PM version of the code to treat a generic power-law pair potential with a core. As in the original code we use a soft repulsive core, with compact support: for $r < \epsilon$ $V(r)$ decreases continuously to a minimum at $r \approx \epsilon/2$ and then increases back to a local maximum $V(r = 0) = 0$. In what follows the values of ϵ quoted correspond to the separation at which the force is still attractive but has dropped to approximately 30% of its value in absence of smoothing. We consider here the attractive case (i.e. $g < 0$). The simulations are checked using simple convergence tests on the numerical parameters, and their accuracy is monitored using energy conservation. For the time steps used here it is typically of order 0.1% over the whole run, orders of magnitude smaller than the typical variation of the kinetic or potential energy over the same time. As initial conditions we take the N particles on the sites of a simple cubic lattice of side L_0 and ascribe random velocities uniformly distributed in an interval $[-\Delta, \Delta]$ in each direction (i.e., "water-bag" type initial conditions in phase space). The parameter Δ is chosen so that initial virial ratio is unity, i.e., $2K/|U| = \gamma$. We choose this initial condition because it would be expected to be close to a QSS to which (collisionless) relaxation should occur "gently." The system is enclosed in a cubic box of side $L \approx 2L_0$ (and centered on the same point as the initial cube of particles). Energy conserving "soft" reflecting boundary conditions are used in the dynamics, i.e., at each time step particles which have moved outside the box have the appropriate components of their velocity inverted. The results we report here required runs lasting as long as two weeks on up to 16 processors.

Shown in Fig. 1 is the evolution of the potential energy U as a function of time, for a pair potential with $\gamma = 5/4$ and $\epsilon/L = 0.01$, for the different values of N indicated. We have defined $\tau_{\rm mf} = \sqrt{mL_0^{\gamma+2}/gN}$, which, given that $L_0 \sim R$, is equivalent parametrically to the definition used above, assuming the scaling in Eq. (6). The macroscopic behavior monitored in this plot is clearly very consistent with what
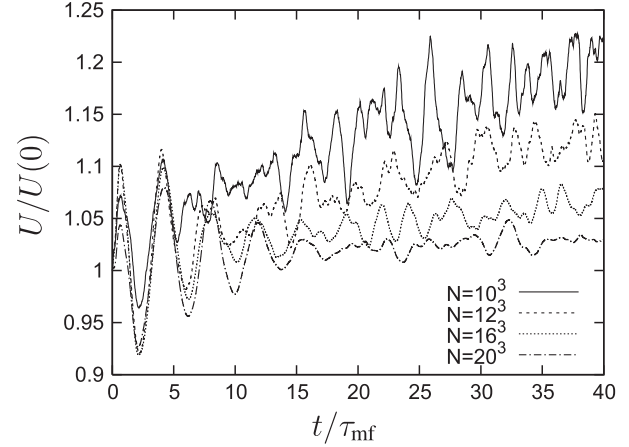

FIG. 1. Temporal evolution of the total potential energy U divided by its initial value $U(0)$, for $\gamma = 1.25$ and a soft core $\epsilon/L = 0.01$, for the different N indicated.

has been anticipated, in line with the typical behavior observed in self-gravitating systems and other systems with long-range interactions studied in the literature: there is a first phase of "violent" (collisionless) relaxation towards an approximate equilibrium, the QSS, which then evolves itself in a second phase on a time scale which clearly depends on N. The first phase, on the other hand, should be N independent: as N increases we see that the different curves are increasingly well superimposed at early times.

Shown in Fig. 2 are, for the two cases $\gamma = 5/4$ and $\gamma = 3/2$, our measurements of the relaxation rate $\Gamma_{\rm relax}$, as a function of N (upper panel) at a chosen fixed ϵ, and as a function ϵ (lower panel) at fixed chosen N. The estimate of $\Gamma_{\rm relax}$ is obtained simply from the slope of the potential energy plotted as a function of time, in the region in each case where this is well fit by a linear behavior, i.e., we take $\Gamma_{\rm relax} = d(\ln U)/dt$ at $t \to 0$. Each point corresponds to one numerical simulation. Note that for these determinations we consider thus only the evolution away from, but still close to, the QSS. Further results on the longer time evolution of these systems, and, in particular, the compatibility of the fully relaxed states with those predicted analytically for this case in [9] (and related numerical studies in [10]) will be given elsewhere.

The upper panel of Fig. 2 includes a line showing the scaling proportional to $1/N$ predicted by Eq. (5) at fixed $b_{\rm min} = \epsilon$. The agreement is clearly very good. Further it is simple to verify that the results are quantitatively very coherent with the prediction: taking $R \approx L_0/2 \approx L/4$, Eq. (5) fit the normalizations of the plot with a prefactor of order unity in both cases. While the degree of this concordance—despite the many approximations which inevitably limit the accuracy we can expect, and the fact that we have dropped all numerical factors in our derivation—is clearly just fortuitous, this quantitative coherence of the results confirms their solidity.

The lower panel of Fig. 2 shows likewise excellent agreement with the predictions above. On it are shown
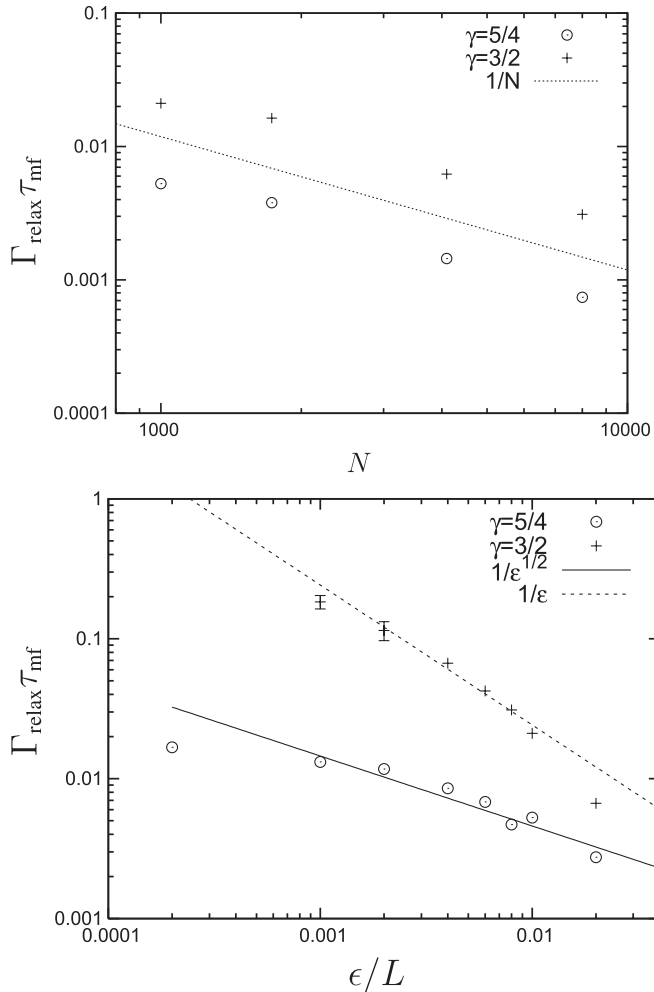
FIG. 2. Estimated relaxation rate Γ_{relax} as a function of N at fixed $\epsilon/L = 0.01$ (upper panel), and as a function of ϵ at fixed $N = 10^3$ (lower panel).

lines corresponding to the behavior of Eq. (5) at fixed N, when we replace $b_{\min}$ by ϵ. As discussed above, this scaling is predicted to be valid in the regime $b_{\min} < \epsilon < b_{\max}$. Below $b_{\min}$ we expect the rates to reach an asymptotic ϵ-independent value of order those estimated in Eq. (8). The behaviors in the plot are very coherent with these predictions, for values of $b_{\min}$ which are in good agreement with Eq. (7), taking again $R \approx L/4$. While we have not predicted the value of $b_{\max}$, the downward deviation (corresponding to a reduction in scattering rate) from the fit at larger ϵ occurs at a value very consistent in each case with the measured mean interparticle distance.

We note that this last plot explains why we consider only γ up to $\gamma = 3/2$, and indeed why we have not tried to verify more directly the scalings in Eq. (8) using simulations with $\epsilon \to 0$. The reason is that, in order to measure the relaxation rates, we need to access the regime $\Gamma_{\text{relax}} \tau_{\text{mf}} \ll 1$, i.e., we need to have a reasonable separation between the times scale of the collisionless dynamics (and formation of QSS) and the relaxation time scale. At $N = 10^3$ we see

that $\gamma = 3/2$ is already at this limit for the smallest ϵ, and the error bars on these points reflect the greater difficulty we have in making the measurement in these cases. The only remedy is to increase N, which, however, is prohibitively expensive numerically, in particular, at small ϵ where the proper integration of the (few) hard collisions included requires significant decrease in the time stepping.

Finally, a few remarks on the relation of these results to some of the extensive recent literature on QSS (see [1] for references). The determination of the N dependence of QSS lifetimes has been much emphasized, both as a target for phenomenological studies of toy models, and for theoretical studies of the problem. Our results show that such lifetimes can be expected to depend, in general, not just on N, but also on the parameters characterizing the short distance properties of the potential. While for $\gamma < d - 1$ a limit $\epsilon = 0$ may be defined [and gives the scaling of Eq. (8)], for $\gamma > d - 1$ this is not possible and the scaling of the relaxation rate will depend necessarily on how ϵ scales with N. It would be interesting to extend our numerical simulations to explore the robustness of QSS notably to effects which may come into play in more physically realistic settings: as shown by a recent study [11] of a toy model, the introduction of stochasticity in the dynamics may also destroy QSS. We emphasize that our results here apply only to the particular (albeit broad) class of models considered, and *a priori* not, e.g., to long-range spin models in which there is no equivalent of two-body collisions. It remains an interesting open question to determine in a broader such context the conditions for the existence of QSS on the spatial dependence of the interaction.

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