A strong limit theorem in Kac-Zwanzig model

G Ariel[1] **and E Vanden-Eijnden**[2]

[1] Department of Mathematics, The University of Texas at Austin, Austin, TX 78712, USA

[2] Courant Institute of Mathematical Sciences, New York University, New York, New York 10012, USA

E-mail: ariel@math.utexas.edu, eve2@cims.nyu.edu

Abstract. A strong limit theorem is proved for a version of the well-known Kac-Zwanzig model, in which a "distinguished" particle is coupled to a bath of N free particles through linear springs with random stiffness. It is shown that the evolution of the distinguished particle, albeit generated from a deterministic set of dynamical equations, converges pathwise toward the solution of an integro-differential equation with a random noise term. Both the canonical and micro-canonical ensembles are considered.

AMS classification scheme numbers: 60G35,82C23,82C31

Submitted to: *Nonlinearity*

1. Introduction

Deterministic dynamical systems with a large number of degrees of freedom typically display complicated behavior that often seem random. It is not surprising that the evolution of certain observables in these systems can be approximated by a stochastic process. Results in this direction abound in the literature. Most of these results, however, are of weak convergence-type, i.e., it is shown that the evolution of the observables tends to that of a stochastic process in some distributional sense. It is more surprising that the evolution of some observables in deterministic dynamical systems converges pathwise to that of a stochastic process. The present paper offers a result in this direction within the context of a dynamical system first introduced by Ford, Kac and Mazur [4, 5], and later by Zwanzig [18], as a simplified model to investigate several issues in nonequilibrium statistical mechanics.

Kac-Zwanzig model is an Hamiltonian dynamical system with Hamiltonian:

$$H(\mathbf{x}, \mathbf{v}) = \frac{1}{2}p_0^2 + V(x_0) + \frac{1}{2}\sum_{i=1}^{N} m_i v_i^2 + \frac{\gamma}{2N}\sum_{i=1}^{N}(x_i - x_0)^2, \tag{1.1}$$

where for shorthand we use the notation $\mathbf{x} = (x_0, x_1, \ldots, x_N)$ and similarly for writing vectors in $\mathbb{R}^{N+1}$. Here $x_0(t)$ and $v_0(t)$ denote the position and velocity at time t of a one dimensional, unit mass particle whose dynamics we are interested in describing. This particle, referred to as the distinguished particle, is placed in an external potential $V(\cdot)$ and coupled to N additional particles (or oscillators), referred to as the bath. The position, velocity and mass of the i'th oscillator are denoted $x_i(t)$, $v_i(t)$ and m_i, respectively. The coupling between the distinguished particle and each oscillator is taken as harmonic, with spring constant $\gamma/N > 0$. The scaling with N emphasizes the fact that the pair interactions are weak. The equations of motion derived from the Hamiltonian (1.1) can be written as: for $i = 1, \ldots, N$,

$$\begin{aligned} \ddot{X}_0^N &= f(X_0^N) - \frac{\gamma}{N}\sum_{i=1}^{N}(X_0^N - X_i^N), \; X_0^N(0) = x_0, \; \dot{X}_0^N(0) = v_0 \\ \ddot{X}_i^N &= \omega_i^2(X_0^N - X_i^N), \qquad\qquad X_i^N(0) = x_i, \; \dot{X}_i^N(0) = v_i, \end{aligned} \tag{1.2}$$

where $f(\cdot) = -V'(\cdot)$ and we have defined the frequencies

$$\omega_i^2 = \frac{\gamma}{Nm_i}. \tag{1.3}$$

Kac-Zwanzig model has been the subject of extensive research in both the physics and mathematical literature [3, 6, 7, 9, 10, 11, 12, 14, 16, 17], and it is known that the trajectory of the distinguished particle can be approximated by a stochastic process under specific scaling of the initial conditions for the bath, $\{x_i, v_i\}_{i=1}^N$ and the frequencies, $\{\omega_i\}_{i=1}^N$. The core of these results can be summarized as follows.

Let $\beta > 0$ be a parameter and suppose that, for fixed initial conditions of the distinguished particle, x_0 and v_0, and fixed frequencies, $\{\omega_i\}_{i=1}^N$, the initial conditions for the bath, $\{x_i\}_{i=1}^N$ and $\{v_i\}_{i=1}^N$ are random variables with probability distribution:

$$d\mu_{\beta,\omega}^{x_0,v_0}(x_1, \ldots, x_N, v_1, \ldots, v_N) = Z^{-1}e^{-\beta\bar{H}(\mathbf{x},\mathbf{v})}dx_1 \ldots dx_N dv_1 \ldots dv_N \tag{1.4}$$

where Z is a normalization constant such that $\mu(\mathbb{R}^N \times \mathbb{R}^N) = 1$ and

$$\bar{H}(\mathbf{x}, \mathbf{v}) = \frac{\gamma}{2N}\sum_{i=1}^{N}\left(\frac{v_i^2}{\omega_i^2} + (x_i - x_0)^2\right). \tag{1.5}$$

The distribution (1.4) is the marginal (at $x_0, v_0, \{\omega_i\}_{i=1}^N$ fixed) of the Boltzmann-Gibbs canonical distribution associated with the Hamiltonian H (here written in terms of the velocities v_i instead of the momenta p_i), which is an invariant measure for Kac-Zwanzig model (1.2). Because of the specific form of the Hamiltonian, (1.4) implies that, for fixed $\{\omega_i\}_{i=1}^N$, $\{x_i\}_{i=1}^N$ and $\{v_i\}_{i=1}^N$ are independent Gaussian variables with mean x_0 and 0 and variance $N/\beta\gamma$ and $N\omega_i^2/\beta\gamma$, respectively. For convenience we define

$$h_i = \sqrt{\frac{\beta\gamma}{N}}(x_i - x_0); \qquad g_i = \sqrt{\frac{\beta\gamma}{N{\omega_i}^2}}v_i. \tag{1.6}$$

With this definition, $\{h_i\}_{i=1}^N$ and $\{g_i\}_{i=1}^N$ are independent, normally distributed random variables (i.e., Gaussian with zero mean and unit variance).

Suppose in addition that the frequencies $\{\omega_i\}_{i=1}^N$ are independent and identically distributed (i.i.d.) random variables, absolutely continuous with respect to the Lebesgue measure on $[0, \infty)$, and with probability density $p(\cdot)$. We assume that $p(\omega) > 0$ in a connected support and has a finite second moment. Then, as $N \to \infty$, the trajectory of the distinguished particle in phase-space, $\{X_0^N(t), \dot{X}_0^N(t)\}$, converges weakly to the solution of the following integro-differential equation with random noise called a generalized Langevin equation:

$$\ddot{X}_0 = f(X_0) - \int_0^t R(t-\tau)\dot{X}_0(\tau)d\tau + \frac{1}{\sqrt{\beta}}\xi(t), \tag{1.7}$$

where the memory kernel $R : [0, \infty) \mapsto \mathbb{R}$ is given by

$$R(t) = \gamma \int_0^\infty p(\omega)\cos(\omega t)d\omega, \tag{1.8}$$

and $\xi : [0, \infty) \mapsto \mathbb{R}$ is a Gaussian random function with mean zero and covariance $R(\cdot)$. This implies that, given any smooth function with compact support $\phi \in C_0^\infty(\mathbb{R} \times \mathbb{R})$ and for any $T < \infty$, we have that, as $N \to \infty$,

$$\sup_{0 \le t \le T} \left| \mathbf{E}_\omega \mathbf{E}_\mathrm{c}^\omega \left[\phi(X_0^N(t), \dot{X}_0^N(t)) \right] - \mathbf{E}_\xi \left[\phi(X_0(t), \dot{X}_0(t)) \right] \right| \to 0, \tag{1.9}$$

where $\mathbf{E}_\mathrm{c}^\omega[\cdot]$ denotes expectation of the initial condition of the bath with respect to the canonical distribution (1.4) at $\{\omega_i\}_{i=1}^N$ fixed, $\mathbf{E}_\omega[\cdot]$ the expectation with respect to the statistics of the frequencies, and $\mathbf{E}_\xi$ the expectation with respect to the statistics of the noise $\xi(\cdot)$.

As mentioned earlier, the purpose of this paper is to offer a stronger convergence result, namely the pathwise convergence of $\{X_0^N(t), \dot{X}_0^N(t)\}$ toward $\{X_0(t), \dot{X}_0(t)\}$ as $N \to \infty$. This falls under the general strategy of the Skorokhod embedding theorem (c.f. [2], Theorem 13.28) which states that every sequence of stochastic processes that converge in law can be realized on a common probability space in a way such that the new sequence will converge almost surely or strongly. This paper offers an explicit construction for such an embedding for the problem at hand. We note that one such strong convergence result has already been proven by Stuart and Warren [16] who considered a variant of this model in which the frequencies are not random but rather are fixed to be $\omega_i = i$. It is then proven that in the limit $N \to \infty$, and on a fixed time segment $t \in [0, \pi]$, the solution $X_0^N(t)$ and $\dot{X}_0^N(t)$ of (1.2) converges in $L^2(0, \pi)$ to the solution of a limiting equation of the form of (1.7) in which $\xi(t)$ is the time derivative of a Brownian bridge of $[0, \pi]$, i.e.,

$$\mathbf{E}_{g,h}\left[\int_0^\pi \left\{ \left(X_0^N(t) - X_0(t)\right)^2 + \left(\dot{X}_0^N(t) - \dot{X}_0(t)\right)^2 \right\} dt \right] \le \frac{C(T, x_0, v_0)}{N^{1-\epsilon}}, \tag{1.10}$$

for any $\epsilon > 0$. The Brownian bridge is constructed as a geometric series with coefficients $\{h_i\}_{i=1}^\infty$ and $\{g_i\}_{i=1}^\infty$.

In contrast, in the model considered here, the frequencies $\{\omega_i\}_{i=1}^\infty$ are random. This requires a new approach to represent the limiting random noise $\xi(t)$. The precise statement of our result, and the assumptions under which it holds are given in section 2.

However, it can be roughly stated as follows. Given the density $p(\cdot)$, it is possible to represent the Gaussian noise $\xi(\cdot)$ as

$$\xi(t) = \sqrt{\gamma}\int_0^\infty p^{1/2}(\omega)\left(\cos\omega t\ dh_\omega + \sin\omega t\ dg_\omega\right). \tag{1.11}$$

where h_ω and g_ω are two independent copies of the standard Brownian motion on $[0,\infty)$. Using the Itô isometry it is easy to see that $\xi(t)$ is indeed a Gaussian process with zero mean and covariance

$$\mathbf{E}_{g,h}\left[\xi(t_1)\xi(t_2)\right] = \gamma\int_0^\infty p(\omega)\cos\omega(t_1-t_2)d\omega = R(t_1-t_2). \tag{1.12}$$

where $\mathbf{E}_{g,h}[\cdot]$ denotes expectation over the statistics of the Brownian motions h_ω and g_ω. Now, let us denote

$$\bar\omega_i = P^{-1}(i/N), \tag{1.13}$$

where $P^{-1}(z)$ is the inverse function of the distribution of the frequencies, i.e., $P(z) = \int_0^z p(\omega)d\omega$. In addition, given a realization of the frequencies, $\{\omega_i\}_{i=1}^N$, let us denote by $\{\omega_i^*\}_{i=1}^N$ the frequencies obtained from $\{\omega_i\}_{i=1}^N$ by ordering them, i.e., there exists a permutation σ of $\{1,\dots,N\}$ such that $\omega_i^* = \omega_{\sigma(i)}$, $i=1,\dots,N$ and $0\le\omega_i^*\le\omega_2^*\cdots\le\omega_N^*$. Then, as $N\to\infty$, $(X_0^N(t),\dot X_0^N(t))$ converges pathwise toward $(X_0(t),\dot X_0(t))$, the solution of (1.7) with $\xi(\cdot)$ given by (1.11), in the sense that, given any $T\le\infty$,

$$\sup_{0\le t\le T}\mathbf{E}_\omega\mathbf{E}_\mathrm{c}^\omega\mathbf{E}_{g,h}^{(\mathrm{C1})}\left[(X_0^N(t)-X_0(t))^2+(\dot X_0^N(t)-\dot X_0(t))^2\right]\to 0. \tag{1.14}$$

Here $\mathbf{E}_\mathrm{c}^\omega[\cdot]$ and $\mathbf{E}_\omega[\cdot]$ are the expectations defined in (1.9) and $\mathbf{E}_{g,h}^{(\mathrm{C1})}[\cdot]$ denotes the expectation over the statistics of the Brownian motions h_ω, g_ω, conditioned on the event, labeled (C1)

$$\begin{aligned}\sqrt{N}\int_{\bar\omega_{i-1}}^{\bar\omega_i} p^{1/2}(\omega)dh_\omega &= \sqrt{\frac{\beta\gamma}{N}}(x_i^*-x_0) = h_i^*\\ \sqrt{N}\int_{\bar\omega_{i-1}}^{\bar\omega_i} p^{1/2}(\omega)dg_\omega &= \sqrt{\frac{\beta\gamma}{N\omega_i^{*2}}}v_i^* = g_i^*\end{aligned} \tag{1.15}$$

for $i=1,\dots,N$, where the star denoted reordering according to the permutation σ, i.e., $x_i^*=x_{\sigma(i)}$, $v_i^*=v_{\sigma(i)}$, $h_i^*=h_{\sigma(i)}$ and $g_i^*=g_{\sigma(i)}$.

It is not obvious *a priori* how to condition the Brownian motions g_ω and h_ω so that they satisfy (1.15). One of the main results of this paper is the construction of a pair of stochastic processes h_ω^c and g_ω^c that satisfy the constraints (1.15) almost surely, thereby given a precise meaning to this conditioning. This is detailed in section 2.

The precise rate of convergence in (1.14) is given in section 2 (see Theorem 2.2). Theorem 2.3 offers a generalization of this result when the initial condition are distributed microcanonically instead of canonically as in (1.4) – a choice which is more natural in the context of Kac-Zwanzig model. Notice that, unlike (1.9), (1.14) requires that the noise term in the limiting equation (1.7) be related to the initial condition for the bath and the frequencies. It is known that this can always be done, i.e. if (1.9) holds then (1.14) holds for some specific choice of the noise term. Our result, however, is constructive in the sense that it tells explicitly how to pick the noise in the limiting equation (1.7) given the choice of the parameters in the original system (1.2).

The organization of the remainder of this paper is as follows. Section 2 presents the assumptions underlying our model, the strong convergence theorems proved and their implications. Section 3 contains the proof of Theorem 2.2, which holds when the initial conditions of the bath particles are distributed canonically. Section 4 contains the proof Theorem 2.3, which holds when the initial conditions of the bath particles are distributed microcanonically. Finally, in Section 5 we give some concluding remarks and discuss possible extensions and generalizations of the model.

2. Assumptions and main results

Recall a few definitions from the previous Section. Let $P(z)$ denote the distribution function of the frequencies, $P(z) = \int_0^z p(\omega)d\omega$, $P^{-1}(z)$ its inverse, and $\bar{\omega}_i = P^{-1}(i/N)$. Also, given $\{x_i, v_i, \omega_i\}_{i=1}^N$, let $\{\omega_i^*\}_{i=0}^N$ be the frequencies obtained by ordering the ω_i's in ascending order using the permutation σ as explained before and adding $\omega_0^* = 0$ to the set. The random permutation σ can be defined on the space of all permutations of length N (with the discrete σ-algebra). Its probability measure is induced from the measure on N independent copies of the frequencies. Similarly, for fixed N and i, ω_i^* is a random variable defined on the probability space $[0, \infty)^N$ (with the Borel σ-algebra). Furthermore, it is absolutely continuous with respect to the Lebesgue measure. Since all the random variables defined above are derived from $p(\omega)$, we denote expectations with respect to all of their measures by $\mathbf{E}_\omega[\cdot]$. Using the permutation σ, we also denote $\{x_i^* = x_{\sigma(i)}$ and $v_i^* = v_{\sigma(i)}\}_{i=1}^N$. Since the random permutation σ is independent of the initial condition, $\{x_i^*, v_i^*\}_{i=1}^N$ are equal in law to $\{x_i, v_i\}_{i=1}^N$.

Given two independent copies of standard Brownian motion, h_ω and g_ω, define

$$
\begin{aligned}
dh_\omega^\perp &= dh_\omega - \sum_{i=1}^N a_i^h p^{1/2}(\omega)\mathbf{1}_{[\bar{\omega}_{i-1},\bar{\omega}_i)}(\omega)d\omega \\
dg_\omega^\perp &= dg_\omega - \sum_{i=1}^N a_i^g p^{1/2}(\omega)\mathbf{1}_{[\bar{\omega}_{i-1},\bar{\omega}_i)}(\omega)d\omega,
\end{aligned} \tag{2.1}
$$

where

$$
a_i^h = N\int_{\bar{\omega}_{i-1}}^{\bar{\omega}_i} p^{1/2}(\omega)dh_\omega, \qquad a_i^g = N\int_{\bar{\omega}_{i-1}}^{\bar{\omega}_i} p^{1/2}(\omega)dg_\omega \tag{2.2}
$$

and $\mathbf{1}_S(\cdot)$ is the indicator function of the set S, i.e., $\mathbf{1}_S(\omega) = 1$ if $\omega \in S$ and $\mathbf{1}_S(\omega) = 0$ otherwise.

Define also

$$
dH(\omega) = \sum_{i=1}^N b_i^h p^{1/2}(\omega)\mathbf{1}_{[\bar{\omega}_{i-1},\bar{\omega}_i)}(\omega)d\omega
$$

$$dG(\omega) = \sum_{i=1}^{N} b_i^g p^{1/2}(\omega) \mathbf{1}_{[\bar\omega_{i-1},\bar\omega_i)}(\omega) d\omega, \tag{2.3}$$

where

$$b_i^h = \sqrt{N} h_i^*, \qquad b_i^g = \sqrt{N} g_i^*. \tag{2.4}$$

Finally, let

$$\begin{aligned} h_\omega^{\rm c} &= H(\omega) + h_\omega^\perp \\ g_\omega^{\rm c} &= G(\omega) + g_\omega^\perp, \end{aligned} \tag{2.5}$$

Using the Itô isometry, it is easily shown that for almost every choice of $\{\omega_i, x_i, v_i\}_{i=1}^N$

$$\begin{aligned} \mathbf{E}_{g,h}\left[\sqrt{N}\int_{\bar\omega_{i-1}}^{\bar\omega_i} p^{1/2}(\omega) dh_\omega^{\rm c}\right] &= h_i^*, \\ \mathbf{E}_{g,h}\left[\sqrt{N}\int_{\bar\omega_{i-1}}^{\bar\omega_i} p^{1/2}(\omega) dg_\omega^{\rm c}\right] &= g_i^*, \end{aligned} \tag{2.6}$$

and the variance is zero. Hence, denoting by $\mathcal{P}_{g,h}$ the probability space of the two Brownian motions h_ω and g_ω we have that for fixed $\{\omega_i, x_i, v_i\}_{i=1}^N$, the function $h_\omega^{\rm c}$ and $g_\omega^{\rm c}$ satisfy (1.15) $\mathcal{P}_{g,h}$-almost surely, i.e.,

$$\sqrt{N}\int_{\bar\omega_{i-1}}^{\bar\omega_i} p^{1/2}(\omega) dh_\omega^{\rm c} = h_i^*, \qquad \sqrt{N}\int_{\bar\omega_{i-1}}^{\bar\omega_i} p^{1/2}(\omega) dg_\omega^{\rm c} = g_i^*. \tag{2.7}$$

On the other hand, if $\mathcal{P}_{\rm c}^\omega$ denotes the probability space of the bath initial conditions $\{x_i, v_i\}_{i=1}^N$ equipped with the canonical distribution (1.4), $\mathcal{P}_\omega$ the probability space of the N independent frequencies $\{\omega_i\}_{i=1}^N$, each equipped with the probability distribution $p(\omega)d\omega$, we also have:

Lemma 2.1. *$\mathcal{P}_\omega$-almost surely for every $\{\omega_i\}_{i=1}^N$, $h_\omega^{\rm c}$ and $g_\omega^{\rm c}$ are two independent Brownian motions defined on the product space $\mathcal{P}_{g,h} \times \mathcal{P}_{\rm c}^\omega$.*

Proof: It is easily verified that $h_\omega^{\rm c}$ is a Gaussian process with zero mean. In addition, a direct calculation shows that $\mathbf{E}_\omega \mathbf{E}_{\rm c}^\omega \mathbf{E}_{g,h}[h_{\omega_1}^{\rm c} h_{\omega_2}^{\rm c}] = \mathbf{E}_{g,h}[h_{\omega_1} h_{\omega_2}] = |\omega_1 - \omega_2|$, and similarly for $g_\omega^{\rm c}$. □

Thus, for fixed $\{\omega_i, x_i, v_i\}_{i=1}^N$, $h_\omega^{\rm c}$ and $g_\omega^{\rm c}$ qualify as Brownian motions conditioned as in (1.15), and they will allow us to now formulate one of our main results.

Define $\xi^{\rm c}(\cdot)$ as

$$\xi^{\rm c}(t) = \sqrt{\gamma}\int_0^\infty p^{1/2}(\omega)\left(\cos\omega t \; dh_\omega^{\rm c} + \sin\omega t \; dg_\omega^{\rm c}\right). \tag{2.8}$$

We have:

Theorem 2.2 (Canonical case)**.** *Assume that the potential $V(\cdot)$ in (1.2) is $\in \mathcal{C}^2(\mathbb{R})$ and that $V'(\cdot)$ is globally Lipschitz. Then, for $T < \infty$ and every choice of initial condition (x_0, p_0) for the distinguished particle, there exists a constant $C(T, x_0, p_0)$, independent of N, such that,*

$$\sup_{0\le t\le T} \mathbf{E}_\omega \mathbf{E}_{\rm c}^\omega \mathbf{E}_{g,h}\left[\left|X_0^N(t) - X_0^{\rm c}(t)\right|^2 + \left|\dot X_0^N(t) - \dot X_0^{\rm c}(t)\right|^2\right] \le \frac{C(T, x_0, v_0)}{N^{2l}}, \tag{2.9}$$

where $X_0^{\rm c}(\cdot)$ is the solution of (1.7) with $\xi(t) = \xi^{\rm c}(t)$ and the rate of convergence, l, depends only on the tail of $p(\omega)$. Let $p(\omega)$ denote a continuously differentiable probability function on $[0,\infty)$ such that for all ω, $p(\omega) > 0$, $p'(\omega) < 0$ and p has a polynomial tail, i.e., $\lim_{\omega\to\infty} \omega^q p(\omega) = D$, for some $q > 3$ and $0 < D < \infty$. Then, we have that $l = (q-1)/(2q)$. If the tail of $p(\omega)$ is exponential or better, then $l = 1/2$.

Unlike most results known in the literature, Theorem 2.2 is a pathwise convergence result. By this we mean that if we pick a set of frequencies and some initial condition for the bath, Theorem 2.2 tells us how to construct a random noise such that the solution of the limiting equation (1.7) remains close to the trajectory of the distinguished particle satisfying (1.2) in the L^2 sense. In fact, Theorem 2.2 implies that this trajectory converges $\mathcal{P}_{g,h} \times \mathcal{P}_\omega \times \mathcal{P}_{\rm c}^\omega$-almost surely towards the solution of the limiting equation as $N \to \infty$, at least on some subsequence.

It is also clear that the convergence result in Theorem 2.2 remains valid if the statistics of the initial condition for the bath are changed. More precisely, the theorem holds if $\{x_i, v_i\}_{i=1}^N$ at $\{\omega_i\}_{i=1}^N$ fixed are not distributed according to the canonical distribution (1.4) but rather according to some other distribution equivalent to (1.4) (i.e. such that (1.4) is absolutely continuous with respect to this new distribution and vice-versa). In this case, however, Lemma 2.1 will not hold in general, i.e. h_ω^c and g_ω^c will not be Brownian motions on $\mathcal{P}_{g,h} \times \mathcal{P}_{\rm c}^\omega$. As a result, the noise term $\xi^c(\cdot)$ may no longer be a zero-mean Gaussian process, which means that the fluctuation-dissipation relation which says that the covariance of $\xi(\cdot)$ is $R(\cdot)$ will be lost as well. We will not consider situations of this type any further here.

Another modification of the statistics of the initial condition of the bath is more natural. Since the Hamiltonian $\bar{H}(\mathbf{x}, \mathbf{v})$ given by (1.5) is left invariant under the dynamics of Kac-Zwanzig model (1.2), it is natural to assume that, given the frequencies $\{\omega_i\}_{i=1}^N$, the initial condition for the bath are distributed according to the distribution (compare (1.4))

$$d\bar{\mu}_{\beta,\omega}^{x_0,v_0}(x_1,\dots,x_N,v_1,\dots,v_N) = \bar{Z}^{-1}\frac{d\sigma(x_1,\dots,x_N,v_1,\dots,v_N)}{|\nabla \bar{H}(\mathbf{x},\mathbf{v})|}, \qquad (2.10)$$

where $\nabla \bar{H} = (\partial\bar{H}/\partial x_1, \dots, \partial\bar{H}/\partial x_N, \partial\bar{H}/\partial v_1, \dots, \partial\bar{H}/\partial v_N)$, $|\cdot|$ is the Euclidean norm in $\mathbb{R}^{2N}$, $d\sigma(x_1,\dots,x_N,v_1,\dots,v_N)$ denotes the surface element (Lebesgue measure) on the constant energy hypersurface $\mathcal{S} = \{(x_1,\dots,x_N,\, v_1,\dots,v_N) : \bar{H}(\mathbf{x},\mathbf{v}) = N/\beta\}$, and $\bar{Z}$ is a normalization constant such that $\bar{\mu}_{\beta,\omega}^{x_0,p_0}(\mathcal{S}) = 1$. The distribution (2.10) is the marginal (at x_0, p_0 fixed) of the microcanonical probability distribution associated with the Hamiltonian (1.1).

Theorem 2.2 can be generalized to the microcanonical situation. To prepare for this result, define

$$h_\omega^{\rm m} = rH(\omega) + h_\omega^\perp, \qquad (2.11)$$

$$g_\omega^{\rm m} = rG(\omega) + g_\omega^\perp, \qquad (2.12)$$

where $H(\cdot)$, $G(\cdot)$, $h_\omega^\perp$ and $g_\omega^\perp$ are as before, and $r \in [0,\infty)$ is a random variable, independent of all previous ones, and with probability density

$$p(r) = C^{-1} r^{2N-1} e^{-\beta N r^2/2}, \qquad C = \int_0^\infty r^{2N-1} e^{-\beta N r^2/2} dr. \tag{2.13}$$

Define also

$$\xi^{\mathrm{m}}(t) = \sqrt{\gamma} \int_0^\infty p^{1/2}(\omega) \left(\cos\omega t \; dh^{\mathrm{m}}_\omega + \sin\omega t \; dg^{\mathrm{m}}_\omega\right). \tag{2.14}$$

Then we have

Theorem 2.3 (Microcanonical case)**.** *For all $T < \infty$ and every choice of initial condition (x_0, p_0) for the distinguished particle, there exists a constant $C(T, x_0, p_0)$, independent of N, such that,*

$$\sup_{0\le t\le T} \mathbf{E}_\omega \mathbf{E}^\omega_{\mathrm{m}} \mathbf{E}_r \mathbf{E}_{g,h} \left[\left| X^N_0(t) - X^{\mathrm{m}}_0(t) \right|^2 + \left| \dot{X}^N_0(t) - \dot{X}^{\mathrm{m}}_0(t) \right|^2 \right] \le \frac{C(T, x_0, v_0)}{N^{2l}}, \tag{2.15}$$

where $X^{\mathrm{m}}_0(\cdot)$ is the solution of (1.7) with $\xi(t) = \xi^{\mathrm{m}}(t)$ and the rate of convergence, l, is as in Theorem 2.2.

The remainder of this paper is devoted to proving the statements made in this section.

3. The canonical case

In this Section we prove Theorem 2.2, relative to the cases in which the bath initial conditions are distributed according to the canonical distribution (1.4). Most authors studying the Kac-Zwanzig model consider only the canonical ensemble [6, 7, 9, 10, 11, 12, 14, 15, 16, 17].

We begin with a few preliminary calculations. Using either variation of parameters or the Laplace transform, (1.2) can be solved for $X^N_1 \dots X^N_N$. Substituting into the equation for $X^N_0(t)$ and integrating by parts, the equation for $X^N_0(t)$ can be written as

$$\ddot{X}^N_0 = f(X^N_0) - \int_0^t R_N(t-\tau) \dot{X}^N_0(\tau) d\tau + \frac{1}{\sqrt{\beta}} \xi_N(t), \tag{3.1}$$

where

$$R_N(t) = \frac{\gamma}{N} \sum_{i=1}^N \cos\omega_i t. \tag{3.2}$$

and $\xi_N(t)$ is given by

$$\xi_N(t) = \sqrt{\beta} \frac{\gamma}{N} \sum_{i=1}^N \left((x_i - x_0)\cos\omega_i t + v_i \frac{\sin\omega_i t}{\omega_i} \right). \tag{3.3}$$

Note that the bath initial conditions appear only in ξ_N. For this reason we will refer to $\xi_N(t)$ as a random noise term. Changing variables into dimensionless, centered coordinates (1.6) the noise term $\xi_N(t)$ can be written as

$$\xi_N(t) = \sqrt{\frac{\gamma}{N}} \sum_{i=1}^{N} (h_i \cos \omega_i t + g_i \sin \omega_i t)$$
$$= \sqrt{\frac{\gamma}{N}} \sum_{i=1}^{N} (h_i^* \cos \omega_i^* t + g_i^* \sin \omega_i^* t)\,, \tag{3.4}$$

where, in the last line, the sums were reordered according to the permutation σ.

We prove Theorem 2.2 in three steps. The first considers convergence of the memory kernel $R_N(t)$. The second step considers the noise, and finally the position and velocity of the distinguished particle. Strong convergence of $X_0^N(t)$ to $X_0^c(t)$ and of $\dot{X}_0^N(t)$ to $\dot{X}_0^c(t)$ is proved in Theorem 2.2. All steps consider a finite time interval $0 \leq t \leq T$, $T < \infty$. The initial conditions of the bath have the Gibbs distribution (1.4). Hence, h_i and g_i, defined by (1.6), are i.i.d. normal random variables (Gaussian with zero mean and variance one).

Lemma 3.1. *For all $T < \infty$ we have,*

$$\sup_{0 \leq t \leq T} \mathbf{E}_\omega \left[(R_N(t) - R(t))^2 \right] \leq \frac{2\gamma^2}{N}, \tag{3.5}$$

and

$$\sup_{0 \leq t \leq T} \mathbf{E}_\omega \left[(R_N(t) - R(t))^4 \right] \leq \frac{16\gamma^4}{N^2}. \tag{3.6}$$

Proof: For fixed time t, the random variable $\cos \omega t$ is bounded. Hence, the law of large numbers implies that $R_N(t)$ converges to its average for almost all ω,

$$\lim_{N\to\infty} R_N(t) = \lim_{N\to\infty} \frac{\gamma}{N} \sum_{i=1}^{N} \cos \omega_i t = \gamma \mathbf{E}_\omega \left[\cos \omega t \right] \equiv R(t). \tag{3.7}$$

In order to find the rate of convergence, we write

$$\mathbf{E}_\omega \left[(R_N(t) - R(t))^2 \right] =$$
$$= \frac{\gamma^2}{N^2} \sum_{i,j=1}^{N} \mathbf{E}_\omega \left[\cos \omega_i t \cos \omega_j t \right] + R^2(t) - 2R(t) \frac{\gamma}{N} \sum_{i=1}^{N} \mathbf{E}_\omega \left[\cos \omega_i t \right]. \tag{3.8}$$

Splitting the double sum to diagonal ($i = j$) and off diagonal terms, using the independence of different ω_i and the definition (3.7) of $R(t)$ we arrive at (3.5). The estimation (3.6) is proven by a similar calculation. □

It is interesting to note that the calculations above imply that $\xi_N(t)$ converges in distribution to $\xi(t)$. The rate of this weaker convergence is always $N^{-1/2}$ and does not depend on the tail of $p(\omega)$.

Next, we show that for all $0 \leq t \leq T < \infty$,

$$\mathbf{E}_\omega \mathbf{E}_{g,h} \left[(\xi_N(t) - \xi^c(t))^2 \right] \leq \frac{C(T)}{N^{2l}}, \tag{3.9}$$

for some $l > 0$ and where the constant $C(T)$ depends only on T and the probability density function $p(\omega)$.

Let

$$k_N = \lfloor N(1 - N^{-a}) \rfloor, \tag{3.10}$$

where $0 \le a < 1/2$ and $\lfloor x \rfloor = \max\{i \in \mathbb{Z} | i \le x\}$. The following Lemmas will be used in proving convergence of the noise. For simplicity, we will only consider a particular case in which the density function of the frequencies $p(\omega)$ is continuously differentiable, strictly positive, monotonically decreasing, and has a polynomial tail, i.e., $\lim_{x\to\infty} \omega^q p(\omega) = D$, for $q > 3$ and some $0 < D < \infty$. In particular, this implies that there exists $\omega_C > 0$ such that, for all $\omega > \omega_C$

$$C\omega^{-q} \le p(\omega) \le D\omega^{-q}, \tag{3.11}$$

for some $C, D > 0$. Other cases can be considered in a similar way. This condition implies that $\mathbf{E}_\omega[\omega^2] < \infty$. Below we use C and D to denote generic constants whose values may vary between expressions.

We have

Lemma 3.2. *For all* $i = 0, \ldots, N-1$

$$\bar{\omega}_i \le \frac{D}{\left(1 - \frac{i}{N}\right)^{1/(q-1)}}. \tag{3.12}$$

Proof:

$$1 - \frac{i}{N} = \int_{\bar{\omega}_i}^{\infty} p(\omega) d\omega \le \int_{\bar{\omega}_i}^{\infty} \frac{D}{\omega^q} d\omega = \frac{D}{\bar{\omega}_i^{q-1}}. \tag{3.13}$$

Solving for $\bar{\omega}_i$ yields (3.12). □

Lemma 3.3. *For all* $i = 1, \ldots, N-1$,

$$|\bar{\omega}_i - \bar{\omega}_{i-1}|^2 \le \frac{C}{N^2 p^2(\bar{\omega}_i)} \tag{3.14}$$

Proof:

$$\frac{1}{N} = \int_{\bar{\omega}_{i-1}}^{\bar{\omega}_i} p(\omega) d\omega \ge C(\bar{\omega}_i - \bar{\omega}_{i-1}) p(\bar{\omega}_i). \tag{3.15}$$

□

Theorem 3.4. *For all* $i = 0, \ldots, N-1$

$$\mathbf{E}_\omega \left[(\bar{\omega}_i - \omega_i^*)^2 \right] \le \frac{D}{N p^2(\bar{\omega}_i)}, \tag{3.16}$$

The term on the right hand side of (3.16) has a form similar to the setup of the Kolmogorov-Smirnov statistics. The proof, detailed in Appendix A, extends some results of Kolmogorov-Smirnov to random variables that are not uniformly distributed.

Lemma 3.5. *For all* $t \le T$

$$\mathbf{E}_\omega \mathbf{E}_{g,h} \left[(\xi_N(t) - \xi^{c}(t))^2 \right] \le C T^2 \left(\frac{1}{N^{2-a(q+1)/(q-1)}} + \frac{1}{N^a} \right). \tag{3.17}$$

Proof: Substituting in the representation for $\xi^{\rm c}(t)$, (2.8), and the representation for $\xi_N(t)$, (3.4), in which we use (2.7) to express h_i^* and g_i^* in terms of $dh_\omega^{\rm c}$ and $dg_\omega^{\rm c}$, we have,

$$\mathbf{E}_\omega \mathbf{E}_{g,h}\left[(\xi_N(t)-\xi^{\rm c}(t))^2\right] = 2\gamma(1-S_N) \tag{3.18}$$

where

$$S_N = \mathbf{E}_\omega \mathbf{E}_{g,h}\left[\left\{\int_{\mathbb{R}} p^{1/2}(x)\cos(xt)dh_x^{\rm c} + \int_{\mathbb{R}} p^{1/2}(x)\sin(xt)dg_x^{\rm c}\right\}\times \right.$$
$$\left.\times\left\{\sum_{i=1}^N\left(\int_{\bar\omega_{i-1}}^{\bar\omega_i} p^{1/2}(x)dh_x^{\rm c}\cos(\omega_i^* t) + \int_{\bar\omega_{i-1}}^{\bar\omega_i} p^{1/2}(x)dg_x^{\rm c}\sin(\omega_i^* t)\right)\right\}\right]. \tag{3.19}$$

Clearly, we need to show that $S_N \to 1$ in the limit $N\to\infty$. Using the Itô isometry yields

$$S_N = \sum_{i=1}^N \mathbf{E}_\omega\left[\int_{\bar\omega_{i-1}}^{\bar\omega_i} p(x)\cos((x-\omega_i^*)t)dx\right]. \tag{3.20}$$

Bounding the cosine by 1 yields an upper bound, $S_N \le 1$. To get a lower bound, we prove that for most i, $(x-\omega_i^*)$ is small, and the cosine is almost one. The reason why $(x-\omega_{\sigma(i)})$ is not small for all i is due to the tail of the density $p(\omega)$. We therefore break the sum into two parts: up to k_N and above. For $i\le k_N$ we use $\cos x \ge 1-x^2/2$. The left over, $k_N < i \le N$, is trivially bounded by -1. The last $N-k_N$ terms in the sum (3.20) contribute

$$\sum_{i=k_N+1}^N \mathbf{E}_\omega\left[\int_{\bar\omega_{i-1}}^{\bar\omega_i} p(x)\cos((x-\omega_i^*)t)dx\right] \ge -\sum_{i=k_N+1}^N \mathbf{E}_\omega\left[\int_{\bar\omega_{i-1}}^{\bar\omega_i} p(x)dx\right]$$
$$= -\frac{N-k_N}{N} = -N^{-a}, \tag{3.21}$$

where we used the fact that $\int_{\bar\omega_{i-1}}^{\bar\omega_i} p(x)dx = 1/N$. The first k_N terms in the sum (3.20) contribute

$$\sum_{i=1}^{k_N} \mathbf{E}_\omega\left[\int_{\bar\omega_{i-1}}^{\bar\omega_i} p(x)\cos((x-\omega_i^*)t)dx\right]$$
$$\ge \sum_{i=1}^{k_N} \mathbf{E}_\omega\left[\int_{\bar\omega_{i-1}}^{\bar\omega_i} p(x)\left(1-(x-\omega_i^*)^2T^2/2\right)dx\right]$$
$$= \frac{k_N}{N} - \frac{T^2}{2}\sum_{i=1}^{k_N}\int_{\bar\omega_{i-1}}^{\bar\omega_i} p(x)\mathbf{E}_\omega\left[(x-\omega_i^*)^2\right]dx. \tag{3.22}$$

For $x\in[\bar\omega_{i-1},\bar\omega_i]$, we have

$$\mathbf{E}_\omega\left[(x-\omega_i^*)^2\right] \le 2(\bar\omega_i-\bar\omega_{i-1})^2 + 2\mathbf{E}_\omega\left[(\bar\omega_i-\omega_i^*)^2\right]. \tag{3.23}$$

Comparing (3.14) with (3.16) we see that the latter is the dominant term. Substituting (3.16) into (3.22), we need to evaluate

$$\frac{1}{N}\sum_{i=1}^{k_N}\frac{1}{Np^2(\bar\omega_i)} \le \frac{C}{N^2}\sum_{i=1}^{k_N}\frac{1}{\left(1-\frac{i}{N}\right)^{2q/(q-1)}}, \tag{3.24}$$

where we used (3.12) to bound $\bar{\omega}_i$. The behavior of the sum in (3.24) can be compared to the integral $\int_0^{1-\delta} x^{-2q/(q-1)}dx$ with $\delta = 1 - k_N/N \leq CN^{-a}$. The integral diverges asymptotically like $\delta^{-(q+1)/(q-1)}$. Substituting into (3.24), the sum is bounded by $CN^{2aq/(q-1)-2}$. Substituting into (3.22) yields (3.17). □

Lemma 3.6. *Strong convergence of noise:*

$$\sup_{0\leq t\leq T} \mathbf{E}_\omega \mathbf{E}_{g,h} \left[(\xi_N(t) - \xi^{\mathrm{c}}(t))^2\right] \leq \frac{CT^2}{N^{2l}}, \tag{3.25}$$

where $l = (q-1)/(2q)$.

Proof: The optimal bound on $\mathbf{E}_\omega \mathbf{E}_{g,h}[(\xi^N(t) - \xi^{\mathrm{c}}(t))^2]$ is obtained by choosing $a = 2 - 2aq/(q-1)$. Taking the supremum over $0 \leq t \leq T$ yields (3.25). □

This concludes our proof for convergence of the noise for the case of a density function $p(\omega)$ with a polynomial tail. Similar calculations can be done with other examples. For instance, with an exponential, square exponential, or a density function that has a compact support, the rate of convergence of the noise is found to be

$$l = \sup_{q>3} \frac{q-1}{2q} = \frac{1}{2}. \tag{3.26}$$

We are now finally in a position for proving Theorem 2.2, which is done using a Gronwall-type argument:

Proof: [Theorem 2.2] Let $(X_0^{\mathrm{c}}(t), V_0^{\mathrm{c}}(t))$ denote the solutions of the limiting equation:

$$\begin{aligned} \dot{X}_0^{\mathrm{c}}(t) &= V_0^{\mathrm{c}}(t) \\ \dot{V}_0^{\mathrm{c}}(t) &= f(X_0^{\mathrm{c}}(t)) - \gamma \int_0^t R(t-\tau) V_0^{\mathrm{c}}(\tau) d\tau + \frac{1}{\sqrt{\beta}} \xi^{\mathrm{c}}(t), \end{aligned} \tag{3.27}$$

and $(X_0^N(t), V_0^N(t))$ the solution of the equations of motion at finite N:

$$\begin{aligned} \dot{X}_0^N(t) &= V_0^N(t) \\ \dot{V}_0^N(t) &= f(X_0^N(t)) - \gamma \int_0^t R_N(t-\tau) V_0^N(\tau) d\tau + \frac{1}{\sqrt{\beta}} \xi_N(t). \end{aligned} \tag{3.28}$$

For shorthand, for the rest of the section we drop the subscript zero from $X_0^N(t)$,$V_0^N(t)$, $X_0^{\mathrm{c}}(t)$ and $V_0^{\mathrm{c}}(t)$. We also write $\mathbf{E}[\cdot]$ for $\mathbf{E}_\omega \mathbf{E}_{g,h}[\cdot]$. We wish to show that

$$\sup_{0\leq t\leq T} \mathbf{E}\left[\left(X^{\mathrm{c}}(t) - X^N(t)\right)^2 + \left(V^{\mathrm{c}}(t) - V^N(t)\right)^2\right] \leq \frac{C(T)}{N^{2l}}. \tag{3.29}$$

The standard way to obtain strong convergence is using the Gronwall inequality. Denote

$$\phi(t) = \mathbf{E}\left[(X^{\mathrm{c}}(t) - X^N(t))^2 + (V^{\mathrm{c}}(t) - V^N(t))^2\right]. \tag{3.30}$$

From the equations for $X^{\mathrm{c}}(t)$ and $X^N(t)$ we have

$$\begin{aligned} &\mathbf{E}\left[(X^{\mathrm{c}}(t) - X^N(t))^2\right] = \mathbf{E}\left[\left(\int_0^t \left(V^{\mathrm{c}}(\tau) - V^N(\tau)\right) d\tau\right)^2\right] \\ &\leq t \int_0^t \mathbf{E}\left[(V^{\mathrm{c}}(\tau) - V^N(\tau))^2 d\tau\right] \leq T \int_0^t \phi(\tau) d\tau, \end{aligned} \tag{3.31}$$

where the last step was obtained using the Jensen inequality. From the equations for $V^{\rm c}(t)$ and $V^N(t)$ we obtain

$$\begin{aligned}&\mathbf{E}\left[(V^{\rm c}(t)-V^N(t))^2\right]=\\&\mathbf{E}\left[\left\{\int_0^t\left\{f(X^{\rm c}(s))-f(X^N(s))+\beta^{-1/2}\left(\xi^{\rm c}(s)-\xi_N(s)\right)\right.\right.\right.\\&\left.\left.\left.+\gamma\int_0^s\left(R(s-\tau)V^{\rm c}(\tau)-R_N(s-\tau)V^N(\tau)\right)d\tau\right\}ds\right\}^2\right]\end{aligned}\tag{3.32}$$

Using $(a+b+c)^2\le 3(a^2+b^2+c^2)$, we need to control three terms. Since $f(x)$ is uniformly Lipschitz, the first is bound by

$$\mathbf{E}\left[\int_0^t\left\{f(X^{\rm c}(t))-f(X^N(t))\right\}^2dt\right]\le DT\int_0^t\phi(s)ds.\tag{3.33}$$

Note that, as before, D denotes a generic constant. Using (3.25), the second term in (3.32) is

$$\frac{1}{\beta}\mathbf{E}\left[\int_0^t\left(\xi^{\rm c}(s)-\xi_N(s)\right)^2ds\right]\le\frac{DT^2}{N^{2l}}.\tag{3.34}$$

The third term in (3.32) is

$$\begin{aligned}&\gamma^2\mathbf{E}\left[\int_0^t\int_0^s\left\{R(s-\tau)V^{\rm c}(\tau)-R_N(s-\tau)V^N(\tau)\right\}^2d\tau ds\right]\\&\le 2\gamma^2\mathbf{E}\left[\int_0^t\int_0^s R_N^2(s-\tau)\left(V^{\rm c}(\tau)-V^N(\tau)\right)^2d\tau ds\right]\\&\quad+2\gamma^2\mathbf{E}\left[\int_0^t\int_0^s\left(V^{\rm c}(\tau)\right)^2\left(R(s-\tau)-R_N(s-\tau)\right)^2d\tau ds\right]\\&\le 2\gamma^4T^2\int_0^t\int_0^s\phi(\tau)d\tau ds+2\gamma^2\left\{\int_0^t\int_0^s\mathbf{E}\left[\left(V^{\rm c}(\tau)\right)^4d\tau ds\right]\right\}^{1/2}\\&\quad\times\left\{\int_0^t\int_0^s\mathbf{E}\left[\left(R(s-\tau)-R_N(s-\tau)\right)^4\right]d\tau ds\right\}^{1/2},\end{aligned}\tag{3.35}$$

where, in the last line we used the fact that $R_N(t)$ is bounded by γ and the Cauchy-Schwartz inequality. Using a Gronwall inequality argument, similar to the one used for ϕ, one can show that $\mathbf{E}[(V^{\rm c}(t))^4]$ is bounded. In addition, using the estimate (3.6) on the fourth moment of $|R(t)-R_N(t)|$, the last term in (3.35) is bounded by DT/N.

Combining the above bounds for the three terms in (3.32) yields

$$\phi(t)\le D(T)\left[\int_0^t\int_0^s\phi(\tau)d\tau ds+\int_0^t\phi(s)ds+\frac{1}{N^{2l}}\right],\tag{3.36}$$

with initial conditions $\phi(0)=\dot{\phi}(0)=0$. Here, $D(T)$ is polynomial in T. The following is a second order generalization of Gronwall's inequality:

Lemma 3.7. *Let $0\le T<\infty$. Then, for all $t\in[0,T]$ we have that*

$$\phi(t)\le\frac{C_1(T)}{N^{2l}}e^{C_2(T)},\tag{3.37}$$

for some $C_1(T),C_2(T)>0$ independent of N and polynomial in T.

Proof: Let $\psi(t)$ be a non-negative function that satisfies $\ddot{\psi} = A\dot{\psi} + B\psi + C$ with initial conditions $\psi(0) = \dot{\psi}(0) = 0$. Solving for ψ, it is easily verified that $\psi(t) \leq C_3 C e^{C_4 t}$ for some $C_3, C_4 > 0$. Denoting $\eta(t) = \int_0^t \int_0^s \phi(\tau) d\tau ds$, we have that $\ddot{\eta} \leq D\dot{\eta} + D\eta + DN^{-2l}$. Hence, $\eta(t) \leq \psi(t)$. Differentiating twice and taking the supremum in $t \in [0, T]$ yields (3.37).

This concludes the proof of Theorem 2.2. □

Remark: Lemma 5 implies that in the limit $N \to \infty$, the i'th largest frequency, ω_i^*, tends towards $\bar{\omega}_i$. The L^2 convergence rate is also calculated. This suggests another representation for $\xi(t)$, in which $\bar{\omega}_i$ is replaced by w_i^*. This representation will also satisfy Theorem 2.2. Let us denote by

$$\begin{aligned} d\tilde{h}_\omega^\perp &= dh_\omega - \sum_{i=1}^N \tilde{a}_i^h p^{1/2}(\omega) \mathbf{1}_{[\omega_{i-1}^*, \omega_i^*)}(\omega) d\omega \\ d\tilde{g}_\omega^\perp &= dg_\omega - \sum_{i=1}^N \tilde{a}_i^g p^{1/2}(\omega) \mathbf{1}_{[\omega_{i-1}^*, \omega_i^*)}(\omega) d\omega, \end{aligned} \tag{3.38}$$

where

$$\tilde{a}_i^h = \frac{\int_{\omega_{i-1}^*}^{\omega_i^*} p^{1/2}(\omega) dh_\omega}{\int_{\omega_{i-1}^*}^{\omega_i^*} p(\omega) d\omega}, \qquad \tilde{a}_i^g = \frac{\int_{\omega_{i-1}^*}^{\omega_i^*} p^{1/2}(\omega) dg_\omega}{\int_{\omega_{i-1}^*}^{\omega_i^*} p(\omega) d\omega}. \tag{3.39}$$

Define also

$$\begin{aligned} d\tilde{H}(\omega) &= \sum_{i=1}^N \tilde{b}_i^h p^{1/2}(\omega) \mathbf{1}_{[\omega_{i-1}^*, \omega_i^*)}(\omega) d\omega \\ d\tilde{G}(\omega) &= \sum_{i=1}^N \tilde{b}_i^g p^{1/2}(\omega) \mathbf{1}_{[\omega_{i-1}^*, \omega_i^*)}(\omega) d\omega, \end{aligned} \tag{3.40}$$

where

$$\tilde{b}_i^h = \frac{h_i^*}{\left(\int_{\omega_{i-1}^*}^{\omega_i^*} p(\omega) d\omega\right)^{1/2}}, \qquad \tilde{b}_i^g = \frac{g_i^*}{\left(\int_{\omega_{i-1}^*}^{\omega_i^*} p(\omega) d\omega\right)^{1/2}}, \tag{3.41}$$

and

$$\begin{aligned} \tilde{h}_\omega^{\mathrm{c}} &= \tilde{H}(\omega) + \tilde{h}_\omega^\perp \\ \tilde{g}_\omega^{\mathrm{c}} &= \tilde{G}(\omega) + \tilde{g}_\omega^\perp, \end{aligned} \tag{3.42}$$

Finally, let

$$\tilde{\xi}^{\mathrm{c}}(t) = \sqrt{\gamma} \int_0^\infty p^{1/2}(\omega) \left(\cos\omega t \; d\tilde{h}_\omega^{\mathrm{c}} + \sin\omega t \; d\tilde{g}_\omega^{\mathrm{c}}\right). \tag{3.43}$$

Then, we have the following Lemma and Theorem, analog to the case considered in Theorem 2.2.

Lemma 3.8. *$\mathcal{P}_\omega$-almost surely for every $\{\omega_i\}_{i=1}^N$, $\tilde{h}_\omega^{\mathrm{c}}$ and $\tilde{g}_\omega^{\mathrm{c}}$ are two independent Brownian motions defined on the product space $\mathcal{P}_{g,h} \times \mathcal{P}_{\mathrm{c}}^\omega$.*

Theorem 3.9. *For all $T < \infty$ and every choice of initial condition x_0, p_0 for the distinguished particle, there exists a constant $C(T, x_0, p_0)$, independent of N, such that,*

$$\sup_{0\le t\le T} \mathbf{E}_\omega \mathbf{E}_{\mathrm{c}}^\omega \mathbf{E}_{g,h} \left[(X_0^N(t) - \tilde{X}_0^{\mathrm{c}}(t))^2 + (\dot{X}_0^N(t) - \dot{\tilde{X}}_0^{\mathrm{c}}(t))^2 \right] \le \frac{C(T, x_0, v_0)}{N^{2l}}$$

where $\tilde{X}_0^{\mathrm{c}}(\cdot)$ is the solution of (1.7) with $\xi(t) = \tilde{\xi}^{\mathrm{c}}(t)$ and the rate of convergence, l, is the same as in Theorem 2.2.

4. The microcanonical case

In this Section we study the microcanonical situation and prove Theorem 2.3. As we will see the proof is a straightforward generalization of that of Theorem 2.2.

Recall that we assume that the initial conditions of the bath are distributed according to the microcanonical distribution, conditioned on the position and velocity of the distinguished particle, x_0 and v_0. This distribution is given by (2.10). Recall the definition of h_ω^{m} and g_ω^{m} in (2.11) and $\xi^{\mathrm{m}}(\cdot)$ in (2.14). Notice the presence of the random variable r in (2.11). The role this variable is to make up for fluctuations in the total energy that exist is the canonical measure, but are absent in the microcanonical one. Let $X_1 \dots X_{2N}$ be independent, normally distributed random variables. Then, $R = \sqrt{X_1^2 + \ldots + X_{2N}^2}/2N$ is a random variable with probability density function (2.13) and the following Lemma holds (compare to Lemma 2.1):

Lemma 4.1. *$\mathcal{P}_\omega$-almost surely for every $\{\omega_i\}_{i=1}^N$, h_ω^{m} and g_ω^{m} are two independent Brownian motions defined on the product space $\mathcal{P}_{g,h} \times \mathcal{P}_r \times \mathcal{P}_{\mathrm{m}}^\omega$.*

Proof: As before, an elementary calculation shows that h_ω^{m} is a Gaussian process with zero mean and, using (1.15), covariance $\mathbf{E}_\omega \mathbf{E}_r \mathbf{E}_{\mathrm{m}}^\omega \mathbf{E}_{g,h}[h_{\omega_1}^{\mathrm{m}} h_{\omega_2}^{\mathrm{m}}] = |\omega_1 - \omega_2|$, where $\mathbf{E}_r$ denotes expectation with respect to (2.13). g_ω^{m} is handled similarly. □

The above Lemma shows that

$$\xi^{\mathrm{m}}(t) = \sqrt{\gamma} \int_0^\infty p^{1/2}(\omega) \left(\cos \omega t \; dh_\omega^{\mathrm{m}} + \sin \omega t \; dg_\omega^{\mathrm{m}} \right) \tag{4.1}$$

is a new realization of the limiting noise $\xi(t)$, i.e., a Gaussian process with zero mean and covariance function $R(t)$.

Proof:[Theorem 2.3] We can follow the exact route detailed in Theorem 2.2 with one small difference. In the canonical case, the constraints (1.15) implied that the noise at fixed N, $\xi_N(t) = -\sqrt{\gamma/N} \sum (h_i \cos \omega_i t + g_i \sin \omega_i t)$ could be identified as ξ^{c}. This does not hold in the microcanonical case. Instead, the correct relation is $r\xi_N(t) = \xi^{\mathrm{m}}$. However, this additional factor of r does not change any of the consequences of the Lemmas proved in Section 3 since $\mathrm{var}[r] = O(N^{-1})$. Hence, the conclusions of Theorem 2.2 remain unchanged. This concludes the proof of Theorem 2.3. □

5. Outlook

The model considered in this paper can be easily generalized to a case in which both the coupling constant γ and the probability density function $p(\omega)$ depend explicitly on N.

Let $\omega_1^N,\dots,\omega_N^N$ denote N independent samples from a distribution with PDF $p_N(\omega)$. Also, denote the coupling coefficient between the distinguished particle and the i'th bath particle by $\gamma_i^N=\gamma(N,\omega_i^N)$. If the product $\gamma(N,\omega)p_N(\omega)$ converge in $L_1(\omega)$ to a limiting function $p(\omega)$, then the cosine transform of $p(\omega)$ is bounded and continuous. We denote $R_N(t)=\int_0^\infty\gamma(N,\omega)p_N(\omega)\cos\omega t d\omega$ and $R(t)=\int_0^\infty p(\omega)\cos\omega t d\omega$. Under the additional assumptions that $\gamma(N,\omega)p_N(\omega)$ converge also in $L_2(\omega)$, and that $\gamma(N,\omega)\le CN$ for some constant $C>0$, it is easily shown that $R_N(t)$ converges to $R(t)$ in $L_2(\omega)$. The proof is the same as in Lemma 3.1. However, the convergence rate may be smaller. Once strong convergence of the covariance function is established, strong convergence of the noise $\xi_N(t)$ and of the trajectory $(X_0^N(t),\dot{X}_0^N(t))$ follows. For instance, Kupferman et al [12] and Stuart et al [15] suggest the following example

$$
\begin{aligned}
p_N(\omega) &= \frac{1}{N^a}\chi_{[0,N^a]}(\omega)\\
\gamma(N,\omega) &= \frac{2\gamma}{\pi}\frac{1}{\alpha^2+\omega^2}N^a,
\end{aligned}
\tag{5.1}
$$

where $\alpha,\gamma>0$ and $0<a<1$. Since $\lim_{N\to\infty}\int p_N(\omega)\gamma(N,\omega)\cos\omega t d\omega=e^{-\alpha|t|}$, the limiting equation is an Ornstein-Uhlenbeck at equilibrium.

If the requirement for $L_1(\omega)$ convergence is removed, the model admits a much larger variety of limiting processes. For instance, taking $p_N(\omega)=N^a/\pi/(N^{2a}+\omega^2)$ and $\gamma_i=N^a$, yields, for any $0<a<1/2$, $R_N(t)=N^a e^{-N^a|t|}\to\delta(t)$. The limiting noise in this example is white and the limiting stochastic process is given by the Langevin equation. Additional parametrization that also lead to a limiting Langevin equation can be found in [8, 18]. These models should not be fundamentally different than the one considered here. They do, however, involve some additional technical difficulties since the limiting noise $\xi(t)$ is a generalized process whose covariance is given by a distribution. Another example is given by Kupferman [10] who suggests $p_N(\omega)=N^{-a}\chi_{[N^{-c},n^{-c}+N^a]}$ and $\gamma_i=N^a\frac{2}{\pi}\Gamma(1-\gamma)\sin(\gamma\pi/2)\omega_i^{\gamma-1}$, where $0<a,c,\gamma<1$ and $\Gamma(z)$ denotes the Euler Gamma function. He then proves that $\int_0^t\xi_N(s)ds$ converges weakly to a fractional Brownian motion with Hurst parameter $H=1-\gamma/2$ [13].

6. Acknowledgements

We wish to thank Jonathan Goodman, Matthias Heymann, Jose Koiller, Andrew Stuart and Paul Wright for useful discussions and suggestions. We are especially grateful to Ray Kapral for sharing his insight on the Kac-Zwanzig model. Partial support from NSF through Grants DMS01-01439, DMS02-09959 and DMS02-39625, and from ONR through Grant N-00014-04-1-0565 is gratefully acknowledged.

Appendix A. Proof of Theorem 3.4

In this Appendix we prove Theorem 3.4, which gives a bound on the variance of $(\omega_i^*-\bar{\omega}_i)$. Recall that, for fixed N, $\omega_1^*,\dots,\omega_N^*$ denote the ordering of N independent samples of frequencies $\{\omega_i\}_{i=1}^N$ with probability density function $p(\omega)$, i.e., $\omega_1^* \leq \omega_2^* \leq \ldots \leq \omega_N^*$. With probability one the frequencies are disjoint. Recall also that $\bar{\omega}_i = P^{-1}(i/N)$. As before, we use C and D to denote generic, positive constants that are independent of N. The values of the constants may change between expressions.

Breiman ([2], Theorem 13.16) gives a proof for the following result:

Proposition 1. *Let $U_1, \ldots, U_N$ denote N independent samples from a random variable, uniformly distributed on $[0,1]$. Let $U_{\sigma(1)}, \ldots, U_{\sigma(N)}$ denote the same set of samples arranged in increasing order. Then, the random variable*

$$D_N = \sqrt{N} \max_{i \leq N} \left|\frac{i}{N} - U_{\sigma(i)}\right|,$$

has a limiting distribution with finite variance.

This implies that,

$$\max_{i \leq N} \mathbf{E}\left[\left(\frac{i}{N} - U_{\sigma(i)}\right)^2\right] \leq \frac{C}{N}. \tag{A.1}$$

Noting that $P(\omega_{\sigma(i)})$ is uniformly distributed in $[0,1]$, $i/N - U_{\sigma(i)} = P(\omega_i^*) - P(\bar{\omega}_i) \sim p(\bar{\omega}_i)(\omega_i^* - \bar{\omega}_i)$. It is therefore expected that $\mathbf{E}_\omega\left[(\omega_i^* - \bar{\omega}_i)^2\right] \leq p^2(\bar{\omega}_i)/N$. The rest of the appendix is dedicated to proving this statement.

For fixed N and $i = 0, \ldots, N-1$ denote $\Delta\omega_i = \omega_i^* - \bar{\omega}_i$. We first prove that the expectation of $(\Delta\omega_i)^2$ exists.

Lemma 2. *For all $i = 0, \ldots, N-1$,*

$$\mathbf{E}_\omega(\Delta\omega_i)^2 < \infty. \tag{A.2}$$

Proof: Since $\omega_i^* \leq \omega_N^*$, it is sufficient to show that $\mathbf{E}_\omega[(\omega_N^*)^2] < \infty$. Denote the density of the random variable ω_N^* by $p_N^*(\omega)$. We have,

$$P[w_N^* \leq x] = \left(P[w_1 \leq x]\right)^N = \left(\int_0^x p(\omega)d\omega\right)^N. \tag{A.3}$$

Hence,

$$p_N^*(x) = Np(x)\left(\int_0^x p(\omega)d\omega\right)^{N-1}. \tag{A.4}$$

This implies that,

$$\begin{aligned}
\mathbf{E}_\omega[(\omega_N^*)^2] &= \int_0^\infty x^2 p_N^*(x)dx = N\int_0^\infty x^2 p(x)\left(\int_0^x p(\omega)d\omega\right)^{N-1} dx \\
&\leq N\int_0^\infty x^2 p(x)\left(\int_0^\infty p(\omega)d\omega\right)^{N-1} dx \\
&= N\int_0^\infty x^2 p(x)dx < \infty. \qquad \text{(A.5)}
\end{aligned}$$

□

Let $f_i : [0,\infty) \to [-i/N, 1-i/N)$ be defined by

$$f_i(x) = P(x) - \frac{i}{N}. \tag{A.6}$$

It is a monotonically increasing function of x and hence invertible. Let $\Delta P_i = \sqrt{N} f_i(\omega_i^*)$. Since $f_i^{-1}(\omega)$ is uniformly distributed on $[-i/N, 1-i/N]$, then the Kolmogorov -Smirnof theorem implies that ΔP_i converges in distribution to a Gaussian random variable ΔP_∞. We further define $g_i : [-i/\sqrt{N}, (1-i/N)\sqrt{N}] \to [0, \infty)$ as

$$g_i(z) = N[p(\bar{\omega}_i)]^2 [f_i^{-1}(z/\sqrt{N}) - \bar{\omega}_i]^2. \tag{A.7}$$

Then, $(\Delta\omega_i)^2 = g_i(\Delta P_i)/(N[p(\bar{\omega}_i)]^2)$, and we have

Lemma 3. *For all $i = 0, \ldots, N-1$*

$$\mathbf{E}_\omega[g_i] \leq D. \tag{A.8}$$

Before proving the lemma, we note that it implies

Corollary 4. *For all $i = 0, \ldots, N-1$ we have*

$$\mathbf{E}_\omega(\omega_i^* - \bar{\omega}_i)^2 \leq \frac{D}{N[p(\bar{\omega}_i)]^2}. \tag{A.9}$$

This proves Theorem 3.4.

Proof: (lemma 3). Lemma 2 implies that there exist ϵ_i such that

$$\mathbf{E}_\omega g_i(\Delta P_i)\chi_{P_i > (1-i/N)\sqrt{N} - \epsilon_i}(\Delta P_i) < 1. \tag{A.10}$$

Let $I = (-(1-i/N)\sqrt{N} + \epsilon_i, (1-i/N)\sqrt{N} - \epsilon_i)$. We wish to Taylor expand $f_i^{-1}(\Delta P_i/\sqrt{N})$ around $z = 0$ in I. Note that for $i/N < 1/2$, the expansion defines an extension of $f^{-1}(z)$ in $I \cap \{z < -i/N\}$. Recall that $f^{-1}(0) = \bar{\omega}_i$. The first order Taylor expansion together with the residue read

$$f_i^{-1}(\Delta P_i/\sqrt{N}) = \bar{\omega}_i + \frac{1}{p(\bar{\omega}_i)}\frac{\Delta P_i}{\sqrt{N}} - \frac{1}{2}\frac{p'(\tilde{\omega})}{p^2(\tilde{\omega})}\frac{\Delta P_i^2}{N}, \tag{A.11}$$

where $\tilde{\omega}$ is between zero and $\bar{\omega}_i$. Substituting into $g_i(\Delta P_i)$,

$$g_i(\Delta P_i) = \Delta P_i^2 \left[1 - \frac{1}{2}\frac{p'(\tilde{\omega})}{p(\tilde{\omega})}\frac{\Delta P_i}{\sqrt{N}}\right]^2 \leq \Delta P_i^2 \left[2 + \frac{1}{2}\left(\frac{p'(\tilde{\omega})}{p(\tilde{\omega})}\right)^2 \frac{\Delta P_i^2}{N}\right]. \tag{A.12}$$

If the tail of $p(\omega)$ decays polynomially with exponent q then, there exists $C, D > 0$ such that for all $\omega > \bar{\omega}_i$, $p(\omega) > C\omega^{-q}$ and $p'(\omega) < D\omega^{-q}$. This implies that, for $\Delta P_i \geq 0$, $p'(\tilde{\omega})/p(\tilde{\omega}) \leq C\tilde{\omega} \leq C\omega_i^*$. Therefore, for $\Delta P_i \geq 0$,

$$g_i(\Delta P_i) \leq \Delta P_i^2 + \frac{C}{N}(\omega_i^*)^2 \Delta P_i^4. \tag{A.13}$$

From (3.12) we have that for all $i \leq N-1$, $\bar{\omega}_i \leq \bar{\omega}_{N-1} \leq DN^{1/(q-1)}$. Hence, $(\omega_i^*)^2/N \leq 2(\omega_i^* - \bar{\omega}_i)^2/N + 1$, and we have that

$$g_i(\Delta P_i) \leq 2\Delta P_i^2 + \frac{C}{N} g_N \Delta P_i^4, \tag{A.14}$$

In the limit $N \to \infty$, ΔP_i converges in distribution to a Gaussian random variable ΔP_∞. Hence, for large enough N, both $\mathbf{E}_\omega[\Delta P_i^2]$ and $\mathbf{E}_\omega[\Delta P_i^4]$ are bounded by a constant that is independent of i and N. Multiplying (A.14) by $\chi_{\Delta P\geq 0}(\cdot)$ and taking expectations yields

$$\mathbf{E}_\omega[g_i(\Delta P_i)\chi_{\Delta P\geq 0}(\Delta P_i)] \leq C. \tag{A.15}$$

For $\Delta P_i < 0$ the situation is simpler since $\omega_i^* < \bar{\omega}_i$ and

$$|\Delta P_i| = \sqrt{N}\int_{\omega_i^*}^{\bar{\omega}_i} p(\omega)d\omega \geq \sqrt{N}|\omega_i^* - \bar{\omega}_i| \min_{\omega<\bar{\omega}_i} p(\omega). \tag{A.16}$$

Hence,

$$\Delta^2\omega_i = (\omega_i^* - \bar{\omega}_i)^2 \leq \frac{1}{N[\min_{\omega<\bar{\omega}_i} p(\omega)]^2}\Delta P_i^2 \leq \frac{1}{N[p(\bar{\omega}_i)]^2}\Delta P_i^2, \tag{A.17}$$

where we used the fact that $p(\omega)$ is decreasing. Taking expectations yields

$$\begin{aligned}\mathbf{E}_\omega[g_i(\Delta P_i)\chi_{\Delta P_i\leq 0}(\Delta P_i)] &= Np^2(\bar{\omega}_i)\mathbf{E}_\omega[\Delta^2\omega_i\chi_{\Delta P_i\leq 0}(\Delta P_i)] \\ &\leq \mathbf{E}_\omega[\Delta P_i^2] < D,\end{aligned} \tag{A.18}$$

Combining (A.10), (A.15) and (A.18) yields (A.8). □

It is interesting to note that the bound obtained in (A.8) is optimal. Noting that $g_i(z)$ is convex, we have

$$\mathbf{E}_\omega[g_i(\Delta P_i)] \geq g_i(\mathbf{E}_\omega[\Delta P_i]) = g_i([1+o(N)]/\sqrt{N}). \tag{A.19}$$

Expanding in a Taylor series around zero yields

$$\mathbf{E}_\omega[g_i] \geq C. \tag{A.20}$$

[1] G Ariel and E Vanden-Eijnden, Testing Transition State Theory on Kac-Zwanzig Model, J. Stat. Phys. 126 (2007) 43-73.

[2] L Breiman, Probability (1968) Addison-Wesley, Reading.

[3] B Cano and AM Stuart, Underresolved simulations of heat baths, J. Comp. Phys. 169 (2001) 193-214.

[4] GW Ford, M Kac and P Mazur, Statistical mechanics of assemblies of coupled oscillators, J. Math. Phys. 6 (1965) 504-515.

[5] GW Ford and M Kac, On the Quantum Langevin Equation, J. Stat. Phys. 46 (1987) 803-810.

[6] D Givon, R Kupferman and AM Stuart, Extracting macroscopic dynamics: model problems and algorithms, Nonlinearity 17 (2004) R55-R127.

[7] OH Hald and R Kupferman, Asymptotic and numerical analysis for mechanical models of heat baths, J. Stat. Phys. 106 (2002) 1121-1184.

[8] W Huisinga, C Schutte and AM Stuart, Extracting macroscopic stochastic dynamics: model problems, Comm. on Pure Appl. Math. 56 (2003) 234.

[9] S Kim, Brownian motion in assemblies of coupled harmonic oscillators, J. Math. Phys. 15 (1974) 578.

[10] R Kupferman, Fractional Kinetics in Kac-Zwanzig heat bath models, J. Stat. Phys. 111 (2004) 291-326.

[11] R Kupferman and AM Stuart, Fitting SDE models to nonlinear Kac-Zwanzig heat bath models, Physica D-Nonlinear phenomena 199 (2004) 279-316.

[12] R Kupferman, AM Stuart, JR Terry and PF Tupper, Long term behavior of large mechanical systems with random initial data, Stoc. and Dyn. 2 (2002) 533-562.

[13] B Mandelbrot and J van Ness, Fractional Brownian motion, fractional Gaussian noise and applications, SIAM rev. 10 (1968) 422.

[14] H Nakazawa, Quantization of Brownian motion processes in potential fields, Quantum probability and applications II, Lecture notes in mathematics, Editors: A Dold and B Eckmann, Springer, Berlin, (1987) 375-387.

[15] AM Stuart, JR Terry and PF Tupper, Constructing SDEs from ODEs with random data, Stanford University Technical Report SCCM-01-04.

[16] AM Stuart and JO Warren, Analysis and experiments for a computational model of a heat bath, J. Stat. Phys. 97 (1999) 687-723.

[17] Y Zhang, Path-integral formalism for a classical Brownian motion in a general environment, Phys. Rev. E 47 (1993) 3745-3748.

[18] R Zwanzig, Nonlinear Generalized Langevin Equations, J. Stat. Phys. 9 (1973) 215-220.