Journal of Statistical Physics, Vol. 97, Nos. 3/4, 1999

Analysis and Experiments for a Computational Model of a Heat Bath

A. M. Stuart[1,3] and J. O. Warren[2,3]

Received February 23, 1999; final June 9, 1999

A question of some interest in computational statistical mechanics is whether macroscopic quantities can be accurately computed without detailed resolution of the fastest scales in the problem. To address this question a simple model for a distinguished particle immersed in a heat bath is studied (due to Ford and Kac). The model yields a Hamiltonian system of dimension $2N+2$ for the distinguished particle and the degrees of freedom describing the bath. It is proven that, in the limit of an infinite number of particles in the heat bath ($N \to \infty$), the motion of the distinguished particle is governed by a stochastic differential equation (SDE) of dimension 2. Numerical experiments are then conducted on the Hamiltonian system of dimension $2N+2$ ($N \gg 1$) to investigate whether the motion of the distinguished particle is accurately computed (i.e., whether it is close to the solution of the SDE) when the time step is small relative to the natural time scale of the distinguished particle, but the product of the fastest frequency in the heat bath and the time step is not small—the underresolved regime in which many computations are performed. It is shown that certain methods accurately compute the limiting behavior of the distinguished particle, while others do not. Those that do not are shown to compute a different, incorrect, macroscopic limit.

KEY WORDS: Computational statistical mechanics; molecular dynamics; Hamiltonian systems; stiff oscillatory systems; stochastic differential equations; Langevin equation; symplectic methods; energy-conserving methods.

[1] Mathematics Institute, Warwick University, Coventry CV4 7AL, England.

[2] Scientific Computing and Computational Mathematics Program, Gates 288, Stanford University, Stanford, California 94305-9025.

[3] Part of this work was performed while the authors were visitors at the Oxford University Computing Laboratory, England.

0022-4715/99/1100-0687$16.00/0

1. INTRODUCTION

Molecular dynamics models of materials are often characterized by large Hamiltonian systems of ordinary differential equations (ODEs) with broad frequency spectra. For reasons of economy, typical numerical integrations of these systems use the largest possible time steps consistent with numerical stability (boundedness of the computed solution) so that accuracy is not assured for fast time scales in the problem. It is hence of interest to investigate whether macroscopic quantities can nonetheless be computed accurately by such methods. In studying this question an important first step is to identify suitable model problems whose properties are sufficiently well-understood to enable meaningful study of numerical methods applied to it. In Section 2 we describe a simple model, due to Ford and Kac,[9] for the motion of a distinguished particle in a heat bath; the heat bath is modelled by attaching the distinguished particle by linear springs to N other particles. We make a specific choice of spring constants and masses (different from that in ref. 9) for which the motion of the distinguished particle in the limit $N \to \infty$ is governed by a stochastic differential equation (SDE) of Langevin type. Our specific choice of parameters leads to rationally related natural frequencies of the heat bath; this allows a straightforward proof of the existence of limiting $N \to \infty$ behavior for the distinguished particle. We exploit this limiting behavior in the subsequent numerical experiments. Section 3 contains a proof of the limiting behavior. It is worthwhile pointing out that, in contrast to the usual situation in statistical mechanics, we will be concerned here with strong approximation of the macroscopic quantities and hence our theorem concerning limiting behavior is a sample path result; this is the appropriate type of result for the type of investigation of numerical accurcacy which we consider here. However it would also be of interest to study weak approximation properties of numerical methods—see ref. 7 for some work in this direction.

In Section 4 we consider three numerical methods applied to the Hamiltonian system of dimension $2N+2$: a symplectic Euler method, a non-symplectic modification, and the backward Euler scheme. Thus we have three different time-discrete maps approximating the solution operator of a Hamiltonian system of dimension $2N+2$; the first retains the symplectic character of the solution operator while the other two do not. We fix the product of the time step and largest natural frequency at $\mathcal{O}(1)$. The dimension of the problem is then increased $(N \to \infty)$ and the approximating map iterated. The solution is projected onto the variables representing the distinguished particle and then compared with the exact motion of the particle given by the SDE $(N = \infty)$. In this set-up the fastest scales are not accurately resolved by the map and it is of interest to ask whether the (macroscopic) motion of the distinguished particle is, nonetheless, accurately resolved. The results of our experiments show that the symplectic Euler method does correctly resolve the motion of the distinguished particle, whereas the non-symplectic modification does not. The backward Euler method also resolves the motion of the distinguished particle correctly, indicating that this desirable property is not restricted to symplectic methods.

In Section 5 we extend our results to a parameterized family of numerical methods. These methods are constructed to be energy-conserving[4] for the homogeneous part of the heat bath. We show formally that, in the underresolved regime, the computed motion of the distinguished particle approximately satisfies an SDE whose coefficients depend on the parameters defining the method. For certain combinations of parameters this SDE agrees with the true SDE governing the motion of the distinguished particle and these are the methods which compute the correct limiting behavior as $N \to \infty$. For other combinations of parameters the computed SDE limit has different damping (possibly negative) and different initial conditions from the true SDE limit. *Thus a macroscopic limit is computed, but it is the wrong one.*[5] We verify this result with a final experiment to demonstrate that the non-symplectic modification of the symplectic Euler method converges to a limiting SDE representing an incorrect macroscopic limit. Our results are summarized in Section 6 and a discussion of how they relate to others concerning the numerical analysis of stiff oscillatory systems is given.

2. THE MODEL

In this section we describe a simplified model for the statistical mechanics of a heat bath, taken from ref. 9. This model forms the basis of all our numerical experiments. Consider the Hamiltonian for a single distinguished particle with position q, momentum p and unit mass moving in a potential V and attached by linear springs to N harmonic oscillators, each with position u_j, momentum v_j, mass m_j and stiffness k_j:

$$H = \frac{1}{2} p^2 + V(q) + \sum_{j=1}^{N} \left\{ \frac{v_j^2}{2m_j} + \frac{k_j}{2} (u_j - q)^2 \right\} \tag{2.1}$$

[4] More precisely they conserve a quadratic form close to the true energy.

[5] Another interpretation is that a *correct* macroscopic limit is computed for a given discrete model; this may differ from the macroscopic limit for the continuous model.

The Hamiltonian (2.1) gives rise to Hamilton's equations

$$\begin{aligned} \dot{p} &= -V'(q) + \sum_{j=1}^{N} k_j(u_j - q), \\ \dot{q} &= p, \\ \dot{v}_j &= -k_j(u_j - q), \\ \dot{u}_j &= v_j/m_j \end{aligned} \tag{2.2}$$

Throughout this and the next section we assume that V' is globally Lipschitz and V is positive:

$$\begin{Bmatrix} |V'(a) - V'(b)| \leqslant L\,|a-b| \\ V(a) \geqslant 0 \end{Bmatrix} \qquad \forall a, b \in \mathbb{R} \tag{2.3}$$

Under this assumption global existence and uniqueness follow for (2.2). (The global Lipschitz condition simplifies the analysis but is not necessary.) Eliminating the momenta in (2.2) gives

$$\ddot{q} + V'(q) = \sum_{j=1}^{N} k_j(u_j - q), \qquad m_j \ddot{u}_j + k_j(u_j - q) = 0 \tag{2.4}$$

Now define the natural frequencies of the oscillators by $\omega_j^2 = k_j/m_j$ and solve for $u_j(t)$ in terms of q by means of variation of constants; this gives

$$\begin{aligned} u_j(t) &= a_j \cos(\omega_j t) + b_j \sin(\omega_j t) + \omega_j \int_0^t \sin[\omega_j(t-s)]\, q(s)\, ds \\ &= a_j \cos(\omega_j t) + b_j \sin(\omega_j t) + q(t) - \cos(\omega_j t)\, q(0) \\ &\quad - \int_0^t \cos[\omega_j(t-s)]\, \dot{q}(s)\, ds \end{aligned}$$

Substituting into the equation for q in (2.4) gives

$$\ddot{q} + V'(q) + \int_0^t K_N(t-s)\, \dot{q}(s)\, ds = -K_N(t)\, q(0) + Z_N(t) \tag{2.5}$$

where

$$K_N(t) := \sum_{j=1}^{N} k_j \cos(\omega_j t)$$

and

$$Z_N(t) := \sum_{j=1}^{N} k_j[a_j \cos(\omega_j t) + b_j \sin(\omega_j t)]$$

We fix the initial conditions for $q(0)$ and $\dot{q}(0) = p(0)$:

$$q(0) = q_0, \qquad p(0) = p_0$$

Now assume that $u_j(0)$ is given by the "free" Boltzmann distribution with inverse temperature β. Thus $u_j(0)$ is chosen at random from a probability distribution with density proportional to

$$\exp\left\{-\frac{\beta k_j u_j^2}{2}\right\}$$

For simplicity we choose $v_j(0) = 0$; it would also be possible to choose $v_j(0)$ from the "free" Boltzmann distribution without affecting the nature of the results, but choosing $v_j(0) = 0$ allows a simpler presentation. Hence, using the notation $\mathcal{N}(\mu, \sigma)$ to denote a Gaussian with mean μ and variance σ, we have

$$u_j(0) \sim \mathcal{N}\left(0, \frac{1}{\beta k_j}\right)$$

Thus, since $a_j = u_j(0)$ and $b_j = \dot{u}_j(0)/\omega_j$ we have

$$a_j \sim \mathcal{N}\left(0, \frac{1}{\beta k_j}\right), \qquad b_j = 0$$

The idea of ref. 9 is to choose the ω_j from a continuous distribution in such a way that, for large N, the function $Z_N(t)$ formally approximates a Fourier integral representation of white noise. Formally this leads to a Langevin equation for q although no proofs have been given of this limiting behavior for large N (but see ref. 14 for related questions). In contrast, here we choose the ω_j so that $Z_N(t)$ approximates a Fourier *series* representation of white noise: we choose $k_j = \gamma^2$ and $m_j = \gamma^2/j^2$ so that $\omega_j = j$. With this, K_N and Z_N simplify to give

$$K_N(t) = \gamma^2 \sum_{j=1}^{N} \cos(jt),$$
$$Z_N(t) = \frac{\gamma}{\sqrt{\beta}} \sum_{j=1}^{N} \mu_j \cos(jt) \tag{2.6}$$

where $\{\mu_j\}_{j=1}^{\infty}$ are IID random variables distributed as $\mathcal{N}(0, 1)$.

Formally, for $t \in [0, \pi]$, Fourier cosine series show that, for δ_0 the Dirac mass at the origin,

$$\frac{1}{\gamma^2} K_{\mathrm{N}}(t) \approx \pi\delta_0(t) - \frac{1}{2} \tag{2.7}$$

for N large; furthermore $Z_{\mathrm{N}}(t)$ is a Gaussian stochastic process with correlation function

$$\mathbb{E} Z_{\mathrm{N}}(t)\, Z_{\mathrm{N}}(s) = \frac{1}{2\beta}\,[K_{\mathrm{N}}(t+s) + K_{\mathrm{N}}(t-s)]$$

so that, formally, $Z_{\mathrm{N}}(t)$ is closely related to white noise for N large (since white noise is a Gaussian process with delta correlations). Substituting the approximation (2.7) for $K_{\mathrm{N}}(t)$ into (2.5) gives the candidate limit problem

$$\begin{gathered} \ddot{Q} + \frac{\gamma^2\pi}{2}\,\dot{Q} + V'(Q) - \frac{\gamma^2}{2}\,Q = \dot{W} \\ Q(0) = q_0, \qquad \dot{Q}(0) = p_0 - \frac{\gamma^2\pi}{2}\,q_0 \end{gathered} \tag{2.8}$$

We anticipate that $\dot{W}$ (the limit of Z_{N}) will be closely related to white noise so that a precise interpretation of this equation will require reformulation as an integral equation. These ideas are made precise in the next section. There it will be convenient to define definite integrals of K_{N} and Z_{N}, namely

$$\begin{aligned} R_{\mathrm{N}}(t) &:= \gamma^2 \sum_{j=1}^{N} \frac{1}{j} \sin(jt), \\ Y_{\mathrm{N}}(t) &:= \frac{\gamma}{\sqrt{\beta}} \sum_{j=1}^{N} \frac{\mu_j}{j} \sin(jt). \end{aligned} \tag{2.9}$$

3. LIMITING BEHAVIOUR FOR LARGE *N*

Throughout this section, and the remainder of the paper, we consider (2.4) with $k_j = \gamma^2$ and $m_j = \gamma^2/j^2$ so that it reduces to

$$\ddot{q} + V'(q) = \gamma^2 \sum_{j=1}^{N} (u_j - q), \qquad \ddot{u}_j + j^2(u_j - q) = 0 \tag{3.1}$$

The initial conditions are

$$q(0) = q_0, \qquad \dot{q}(0) = p_0,$$
$$u_j(0) \sim \frac{1}{\gamma \sqrt{\beta}}\, \mu_j, \qquad \dot{u}_j(0) = 0 \tag{3.2}$$

with $\mu_j \sim \mathcal{N}(0, 1)$ and IID. Note that with our assumptions about k_j and m_j, $K_{\mathrm{N}}(t)$ and $Z_{\mathrm{N}}(t)$ are given by (2.6) and $R_{\mathrm{N}}(t)$ and $Y_{\mathrm{N}}(t)$ by (2.9).

The purpose of this section is to prove Theorem 3.5 which shows that q solving (3.1), (3.2) for large N is close to Q solving an SDE of the form (2.8).

We define $\bar{R}_{\mathrm{N}}$ by

$$\bar{R}_{\mathrm{N}}(t) = \frac{\gamma^2}{2}\,[\pi - t] - R_{\mathrm{N}}(t)$$

noting that in $L^2(0, \pi)$ it is given by

$$\bar{R}_{\mathrm{N}}(t) = \gamma^2 \sum_{j=N+1}^{\infty} \frac{1}{j} \sin(jt)$$

From this it follows that, for all large N,

$$\|\bar{R}_{\mathrm{N}}(\cdot)\|^2 = \left\| R_{\mathrm{N}}(\cdot) - \frac{\gamma^2}{2}\,[\pi - \cdot\,] \right\|^2 \leqslant \frac{C}{N} \tag{3.3}$$

where $\|\cdot\|$ denotes the $L^2(0, \pi)$ norm. Here and throughout the paper, C denotes a constant independent of N; its actual value may change from occurence to occurence. We let $\|\cdot\|_T$ denote the $L^2(0, T)$ norm for $T \leqslant \pi$. Throughout the remainder of the paper we will assume $T \leqslant \pi$ without comment. By use of Theorem 5, Section 2, Section II in ref. 15 it may be shown that

$$\mathbb{E}\, \| Y_{\mathrm{N}}(\cdot) - W(\cdot)\|^2 \leqslant \frac{C}{N} \tag{3.4}$$

where $W(t)$ is a scaled Brownian bridge on $[0, \pi]$. Specifically,

$$W(t) = \frac{\gamma}{\sqrt{\beta}} \sum_{j=1}^{\infty} \frac{\mu_j}{j} \sin(jt) = \gamma \sqrt{\frac{2}{\pi\beta}} \left[B(t) - \frac{t}{\pi}\, B(\pi) \right] \tag{3.5}$$

where B is standard Brownian motion.

It is also convenient to define $\mathscr{M}: H^1(0, \pi) \to L^2(0, \pi)$ by

$$(\mathscr{M}p)(t) = \bar{R}_N(t)\, p(0) + \int_0^t \bar{R}_N(t-s)\, \dot{p}(s)\, ds$$

noting that

$$\int_0^t K_N(t-s)\, p(s)\, ds = \gamma^2 \left[\frac{\pi}{2}\, p(t) - \int_0^t \frac{p(s)}{2}\, ds \right] - (\mathscr{M}p)(t)$$

With this definition, (2.5), (2.6) and hence (3.1), (3.2) are equivalent to solving

$$\ddot{q} + V'(q) - \frac{\gamma^2}{2}\, q + \frac{\gamma^2 \pi}{2}\, \dot{q} = -\left[\frac{\gamma^2}{2} + K_N(t) \right] q(0) + Z_N(t) + (\mathscr{M}\dot{q})(t),$$
$$q(0) = q_0, \qquad \dot{q}(0) = p_0 \tag{3.6}$$

Since we anticipate that the limit problem is an Itô SDE, we re-introduce the momentum $p(t) := \dot{q}(t)$ and reformulate (3.6) as an integral equation:

$$q(t) = \int_0^t p(s)\, ds + q_0,$$
$$p(t) = \int_0^t \left[\frac{\gamma^2}{2}\, q(s) - \frac{\gamma^2 \pi}{2}\, p(s) - V'(q(s)) \right] ds \tag{3.7}$$
$$+ p_0 - \frac{\gamma^2 \pi}{2}\, q_0 + Y_N(t) + \bar{R}_N(t)\, q_0 + \int_0^t (\mathscr{M}p)(s)\, ds$$

We wish to compare the solution of (3.7) with the Itô SDE

$$Q(t) = \int_0^t P(s)\, ds + q_0,$$
$$P(t) = \int_0^t \left[\frac{\gamma^2}{2}\, Q(s) - \frac{\gamma^2 \pi}{2}\, P(s) - V'(Q(s)) \right] ds + p_0 - \frac{\gamma^2 \pi}{2}\, q_0 + W(t) \tag{3.8}$$

From (3.3) we know that $\bar{R}_N$ is $\mathscr{O}(N^{-1/2})$ in $L^2(0, \pi)$ and (3.4) gives bounds on $(Y_N - W)$. Thus it remains to estimate the integral of $(\mathscr{M}p)(s)$ to show the closeness of solutions to (3.7) and (3.8). We will show that in mean square $\|\mathscr{M}p\| = \mathscr{O}(\ln N/N^{1/2})$. The essential difficulty to overcome is that $\mathbb{E}\,\|\dot{p}\|^2$ is $\mathcal{O}(N)$, so a straightforward Cauchy–Schwarz bound on $\|\mathcal{M}p\|$ is $\mathcal{O}(1)$. Thus we work to exploit some near orthogonality to prove the required bound. This near orthogonality is expressed in Lemma 3.2.

Straightforward calculation shows that

$$\left\|\frac{\gamma^2}{2}+K_{\mathrm{N}}(\cdot)\right\|^2 \leqslant \beta_1 N, \qquad \mathbb{E}\,\|Z_{\mathrm{N}}(\cdot)\|^2 \leqslant \beta_2 N \tag{3.9}$$

Now, if $T<\pi$, by (3.3),

$$\begin{aligned}\int_0^T (\mathcal{M}p)(t)^2\,dt &\leqslant 2\left[\int_0^\pi \bar{R}_{\mathrm{N}}(t)^2\,dt\right] p_0^2 + 2\int_0^T\left[\int_0^t \bar{R}_{\mathrm{N}}(t-s)\,\dot{p}(s)\,ds\right]^2 dt\\ &\leqslant \frac{2C}{N}\,p_0^2+\frac{2\pi C}{N}\,\|\dot{p}\|_T^2\end{aligned} \tag{3.10}$$

We use this to show the following preliminary lemma:

Lemma 3.1. The solution of (3.6) satisfies, for all N sufficiently large and for $0\leqslant T\leqslant\pi$,

$$\mathbb{E}\,\|\ddot{q}\|_T^2 \leqslant A_1\,\mathbb{E}\,\|\dot{q}\|_T^2 + A_2\,\mathbb{E}\,\|q\|_T^2 + A_3(q_0^2+1)\,N + \frac{A_4}{N}\,p_0^2$$

$$\mathbb{E}\,\|(\mathcal{M}\dot{q})\|_T^2 \leqslant \frac{B_1}{N}\,p_0^2 + B_2(q_0^2+1) + \frac{B_3}{N}\,\mathbb{E}\,\|\dot{q}\|_T^2 + \frac{B_4}{N}\,\mathbb{E}\,\|q\|_T^2$$

Proof. From (3.6) we have

$$\|\ddot{q}\|_T^2 \leqslant C\left\{\|V'(q)\|_T^2 + \|q\|_T^2 + \|\dot{q}\|_T^2 + \left\|\frac{\gamma^2}{2}+K_{\mathrm{N}}(\cdot)\right\|_T^2 q_0^2 + \|Z_{\mathrm{N}}\|_T^2 + \|\mathcal{M}\dot{q}\|_T^2\right\}$$

By (2.3), (3.9) and (3.10) we deduce that

$$\mathbb{E}\,\|\ddot{q}\|_T^2 \leqslant A_1'[1+\mathbb{E}\,\|q\|_T^2] + A_2'\,\mathbb{E}\,\|\dot{q}\|_T^2 + A_3' N q_0^2 + A_4' N + \frac{A_5'}{N}\,p_0^2 + \frac{A_6'}{N}\,\mathbb{E}\,\|\ddot{q}\|_T^2$$

Thus for N sufficiently large the first result follows. By applying this to (3.10) the second result is obtained. ∎

The following lemma, whose proof is given in Appendix 1, will enable us to prove the improved bound on $\mathbb{E}\,\|(\mathcal{M}\dot{q})\|_T^2$, which follows in Lemma 3.3.

Lemma 3.2. There is a constant $C>0$ such that, for all N sufficiently large and for $0 \leqslant T \leqslant \pi$,

$$\left\| \int_0^t \bar{R}_N(t-s) \left[\frac{\gamma^2}{2} + K_N(s) \right] ds \right\|^2 + \mathbb{E} \left\| \int_0^t \bar{R}_N(t-s)\, Z_N(s)\, ds \right\|^2 \leqslant C\, \frac{(\ln N)^2}{N}$$

Lemma 3.3. The solution of (3.6) satisfies, for all N sufficiently large and for $0 \leqslant T \leqslant \pi$,

$$\mathbb{E}\, \|(\mathscr{M}\, \dot{q})\|_T^2 \leqslant \frac{C}{N} \left[(\ln N)^2 \left\{ 1 + q_0^2 + p_0^2 \right\} + \mathbb{E} \left\{ \|q\|_T^2 + \|\dot{q}\|_T^2 \right\} \right]$$

Proof. By (3.6) we have

$$\begin{aligned}
(\mathscr{M}\dot{q})(t) &= \bar{R}_N(t)\, p_0 + \int_0^t \bar{R}_N(t-s)\, \ddot{q}(s)\, ds \\
&= \bar{R}_N(t)\, p_0 + \int_0^t \bar{R}_N(t-s) \left[\frac{\gamma^2}{2}\, q(s) - V'(q(s)) - \frac{\gamma^2 \pi}{2}\, \dot{q}(s) \right] ds \\
&\quad + \int_0^t \bar{R}_N(t-s) \left[Z_N(s) - \left(\frac{\gamma^2}{2} + K_N(s) \right) q_0 + (\mathscr{M}\dot{q})(s) \right] ds
\end{aligned}$$

Applying (2.3), (3.3) and Lemma 3.1 we deduce that

$$\begin{aligned}
\mathbb{E}\, \|(\mathscr{M}\dot{q})\|_T^2 \leqslant{}& C\, \mathbb{E} \left[\frac{p_0^2}{N} + \frac{1+q_0^2}{N} + \frac{\|q\|_T^2}{N} + \frac{\|\dot{q}\|_T^2}{N} \right] \\
&+ C\, \mathbb{E} \left\| \int_0^t \bar{R}_N(t-s) \left[\frac{\gamma^2}{2} + K_N(s) \right] q_0^2\, ds \right\|_T^2 \\
&+ C\, \mathbb{E} \left\| \int_0^t \bar{R}_N(t-s)\, Z_N(s)\, ds \right\|_T^2
\end{aligned}$$

The required result follows from Lemma 3.2. ∎

We now use Lemma 3.3 to derive some *a priori* bounds on solutions of (3.7) (which is equivalent to (3.6) and hence (3.1), (3.2)).

Lemma 3.4. The solution of (3.7) satisfies, for all N sufficiently large and for $0 \leqslant T \leqslant \pi$,

$$\mathbb{E}\{ \|p\|_T^2 + \|q\|_T^2 \} \leqslant c_1 \exp(c_2 T)[1 + p_0^2 + q_0^2]$$

Proof. From (3.7), using $T<\pi$, it follows that

$$\|q\|_T^2 \leqslant C\left[q_0^2 + \int_0^T \|p\|_t^2 \, dt \right]$$

Similarly from (3.7), using (2.3) and (3.3),

$$\|p\|_T^2 \leqslant C\left[1 + p_0^2 + q_0^2 + \|Y_{\mathrm{N}}\|_T^2 + \int_0^T \|\mathscr{M}p\|_t^2 \, dt + \int_0^T \|q\|_t^2 + \|p\|_t^2 \, dt \right]$$

for all large N. A straightforward calculation reveals that

$$\mathbb{E} \, \|Y_{\mathrm{N}}\|_T^2 \leqslant C$$

and Lemma 3.3 shows that, for all large N,

$$\mathbb{E} \int_0^T \|\mathscr{M}p\|_t^2 \, dt \leqslant C\left[q_0^2 + p_0^2 + \int_0^T \{1 + \mathbb{E} \, \|q\|_t^2 + \mathbb{E} \, \|p\|_t^2\} \, dt \right]$$

Thus, for

$$r(t) := \mathbb{E}\{\|p\|_t^2 + \|q\|_t^2\}$$

we have

$$r(T) \leqslant C\left[1 + p_0^2 + q_0^2 + \int_0^T r(t) \, dt \right]$$

and a Gronwall argument gives the required result. ∎

Remark. The previous lemma shows that q and $\dot{q}$ are bounded independently of N as is to be expected if (3.7) reproduces a limit solving (3.8). Note, however, that Lemma 3.1 gives an (expected) $\mathcal{O}(N^{1/2})$ bound on $\ddot{q}$, again reflecting the fact that the limit problem (3.8) (equivalently (2.8)) has solution with no second derivative.

Finally we may compare (3.7) and (3.8). Note that (3.7) is equivalent to (3.1), (3.2) and (3.8) is the rigorous interpretation of the SDE (2.8). Hence the next theorem relates the solution of a large Hamiltonian system with random initial data to the solution of an SDE. We have:

Theorem 3.5. Under (2.3) the solutions of (3.7) and (3.8) satisfy, for all N sufficiently large and for $0 \leqslant T \leqslant \pi$,

$$\mathbb{E}\{\|q-Q\|_T^2 + \|p-P\|_T^2\} \leqslant c_1 \exp(c_2 T) \frac{(\ln N)^2}{N}$$

and

$$\mathbb{E}\,|q(T)-Q(T)|^2 \leqslant c_1 T \exp(c_2 T)\,\frac{(\ln N)^2}{N}$$

Proof. Let

$$d(t)=q(t)-Q(t), \qquad e(t)=p(t)-P(t)$$

From (3.7) and (3.8) we obtain

$$d(t)=\int_0^t e(s)\,ds,$$

$$e(t)=\int_0^t \left[\frac{\gamma^2}{2}\,d(s)-(V'(q(s))-V'(Q(s))-\frac{\gamma^2\pi}{2}\,e(s)\right] ds$$

$$+\bar{R}_N(t)\,q_0+[Y_N(t)-W(t)]+\int_0^t (\mathscr{M}p)(s)\,ds$$

By (2.3), (3.3), (3.4) and Lemma 3.3 we have, for large N,

$$\mathbb{E}\,\|d\|_T^2 \leqslant C \int_0^T \mathbb{E}\,\|e\|_t^2\,dt,$$

$$\mathbb{E}\,\|e\|_T^2 \leqslant C \int_0^T \left[\mathbb{E}\,\|d\|_t^2+\mathbb{E}\,\|e\|_t^2+\frac{(\ln N)^2}{N}\right] dt$$

and so, by a Gronwall argument, the first result follows. The second is obtained from the definition of the error in the position as an integral in time of the momentum. ∎

Remark. The limiting equation satisfied by the u_j as $N \to \infty$ may also be found. Let U_j solve

$$\ddot{U}_j+j^2(U_j-Q)=0,$$

$$U_j(0)=u_j(0), \qquad \dot{U}_j(0)=0$$

Then

$$u_j(t)-U_j(t)=q(t)-Q(t)-\int_0^t \cos[j(t-s)][\dot{q}(s)-\dot{Q}(s)]\,ds$$

Applying Theorem 3.5 shows that

$$\mathbb{E}\,|u_j(T)-U_j(T)|^2 \leqslant 4c_1 T \exp(c_2 T)\,\frac{(\ln N)^2}{N}$$

and

$$\mathbb{E}\,|\dot{u}_j(T)-\dot{U}_j(T)|^2 \leqslant j^2 c_1 T \exp(c_2 T)\,\frac{(\ln N)^2}{N}$$

Thus positions converge pointwise for all j while velocities are only guaranteed to converge for $j=o(N^{1/2}/\ln N)$. ▮

4. NUMERICAL EXPERIMENTS

Theorem 3.5 shows that the solutions $(\dot{q}, q)$ of the Hamiltonian system (3.1), (3.2) with $N \gg 1$ are close, in mean square, to solutions $(\dot{Q}, Q)$ of the formal SDE (2.8), with precise interpretation as the integral equation (3.8) and $W(t)$ given by (3.5). The initial conditions (3.2) for (3.1) depend upon the IID random variables $\{\mu_j\}_{j\geqslant 1}$ appearing in (3.5). For convenience we define

$$a_j := \frac{1}{\gamma\sqrt{\beta}}\,\mu_j$$

The question we wish to address in this section is the following: imagine that we have the solution $(\dot{Q}, Q)$ of the SDE (2.8) with "white noise" given by the derivative of (3.5). Now fix $N \gg 1$ and solve the Hamiltonian system (3.1), (3.2) numerically with time step Δt, taking the μ_j from the white noise expansion. We would like to know whether, under the limiting process

$$N\,\Delta t = \zeta, \qquad \Delta t \to 0, \qquad N \to \infty \tag{4.1}$$

the projection of the numerical solution onto $(\dot{q}, q)$ co-ordinates is close to $(\dot{Q}, Q)$. This corresponds to the situation in which the fast scales of (3.1), (3.2) are not accurately resolved, since the fastest natural frequency of the heat bath is $\mathcal{O}(N)$ and $N\,\Delta t = \zeta$.

The three methods we study numerically in this section are an explicit symplectic Euler method, a non-symplectic modification, and the backward Euler method. All methods are formally first order accurate in Δt, for fixed N.

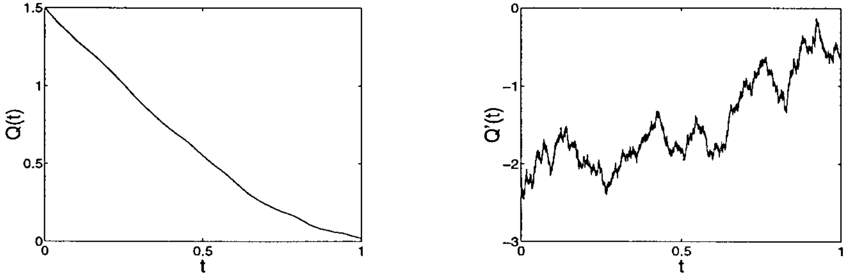

Fig. 1. Exact solutions Q and $\dot{Q}$ for (2.8) with $Q(0) = 1.5$, $\dot{Q}(0) = 0$.

Note, however, that we are interested in taking the limit (4.1) which might be expected to lead to a reduction in accuracy. We first need to find the exact solutions of (2.8). In practice we do this by computing (3.1), (3.2) with $N = 32{,}000$ $(N \approx \infty)$ and $N\,\Delta t = 10^{-3}$ $(\Delta t \approx 0)$. Furthermore we choose

$$V(q) = \tfrac{1}{4}(q^2 - 1)^2 \tag{4.2}$$

and $\gamma = 1$ for all numerical experiments in this paper. Theorem 3.5 and standard ODE convergence results show that this numerical simulation accurately approximates the solution of (2.8) with high probability. The "exact" solutions for Q and $\dot{Q}$ are shown in Fig. 1.

Having constructed the "exact" solution of the limiting SDE we then solve (3.1), (3.2) numerically with $N\Delta t = \zeta$ (precise values of ζ are given for each experiment) and with $N = 2^m \times 10^3$ for $m = 1, 2, 3$ and 4. For each value of m we compute the $L^2(0, t)$ error in $\dot{q}$, comparing with the "exact" solution given in Fig. 1.

With these preliminaries addressed, our first experiment is to apply the symplectic Euler method to (3.1), (3.2):

$$\begin{aligned} u_j^{n+1} &= u_j^n + \Delta t\, v_j^{n+1} \\ v_j^{n+1} &= v_j^n - \Delta t\, j^2(u_j^n - q^n), \\ q^{n+1} &= q^n + \Delta t\, p^{n+1}, \\ p^{n+1} &= p^n - \Delta t\, V'(q^n) + \Delta t\, \gamma^2 \sum_{j=1}^{N} (u_j^n - q^n) \end{aligned} \tag{4.3}$$

where $u_j^n \approx u_j(n\,\Delta t)$ and likewise for the other variables. We fix ζ from (4.1) at 1. The initial conditions are

$$u_j^0 = a_j, \qquad v_j^0 = 0, \qquad q^0 = q_0, \qquad p^0 = p_0 \tag{4.4}$$

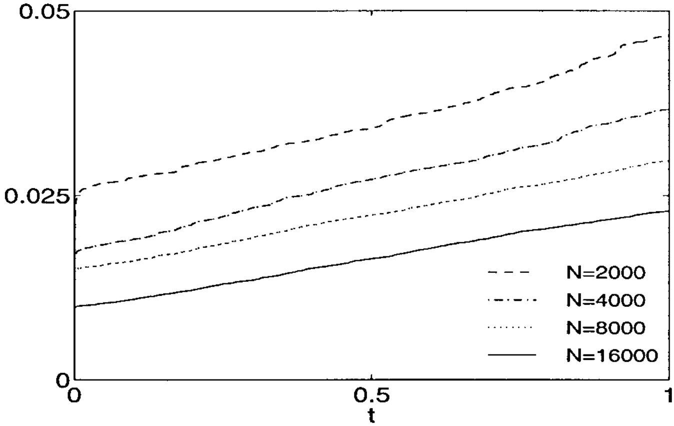

Fig. 2. $L^2(0, t)$ error curves in $\dot{q}(t)$ for symplectic scheme (4.3) compared with SDE limit $\dot{Q}(t)$ from (2.8).

Figure 2 shows the $L^2(0, t)$ error curves in $\dot{q}(t)$ and indicates that the limit SDE is well-approximated by the full Hamiltonian system (3.1), (3.2) with $N\Delta t = 1$. Convergence to the limit is clearly observed under (4.1), showing that macroscopic quantities can be accurately captured without resolution of the fastest scales.

To examine the generality of this property, our second experiment is to slightly modify the previous method in a manner which makes the resulting map non-symplectic:

$$\begin{aligned} u_j^{n+1} &= u_j^n + \Delta t\, v_j^{n+1} \\ v_j^{n+1} &= v_j^n - \Delta t\, j^2(u_j^n - q^n), \\ q^{n+1} &= q^n + \Delta t\, p^{n+1}, \\ p^{n+1} &= p^n - \Delta t\, V'(q^n) + \Delta t\, \gamma^2 \sum_{j=1}^{N} (u_j^{n+1} - q^n) \end{aligned} \tag{4.5}$$

Again we use $\zeta = 1$ and initial conditions (4.4). Figure 3 shows that this method fails to accurately solve for $\dot{Q}$ in (2.8). However, the $L^2(0, t)$ error curves for $\dot{q}$ in Fig. 4 suggest that the numerical solution does converge to some incorrect macroscopic limit under (4.1)—we pursue this further in Section 5.

It is natural to ask whether it is the property of being symplectic which distinguishes between the schemes (4.3) and (4.5). To address this question we apply the backward Euler method, which is not symplectic, and study

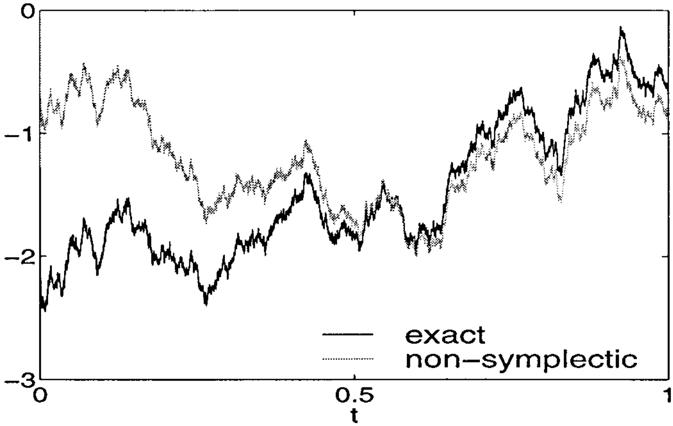

Fig. 3. Exact velocity ($\dot{Q}$) and velocity ($\dot{q}$) computed by non-symplectic scheme (4.5) with $N = 16{,}000$ and $\zeta = 1$.

its error properties. The backward Euler method applied to this model has the following form:

$$\begin{aligned} u_j^{n+1} &= u_j^n + \Delta t\ v_j^{n+1} \\ v_j^{n+1} &= v_j^n - \Delta t\ j^2(u_j^{n+1} - q^{n+1}), \\ q^{n+1} &= q^n + \Delta t\ p^{n+1}, \\ p^{n+1} &= p^n - \Delta t\ V'(q^{n+1}) + \Delta t\ \gamma^2 \sum_{j=1}^{N} (u_j^{n+1} - q^{n+1}) \end{aligned} \tag{4.6}$$

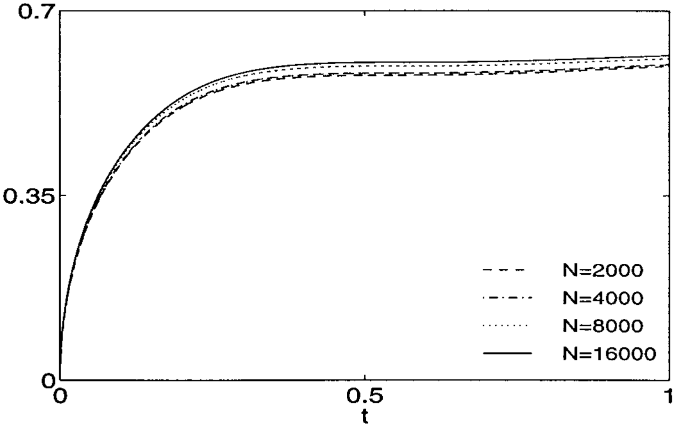

Fig. 4. $L^2(0, t)$ error curves in $\dot{q}(t)$ for non-symplectic scheme (4.5) compared with the SDE limit $\dot{Q}(t)$ from (2.8).

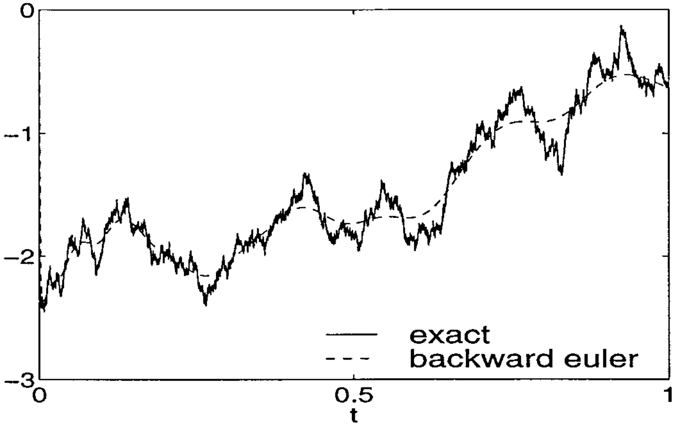

Fig. 5. Exact velocity ($\dot{Q}$) and velocity ($\dot{q}$) computed by the backward Euler method (4.6) with $N = 16,000$ and $\zeta = 10$.

(Note that, in contrast to the previous two methods, this one defines an implicit map from n to $n+1$. In our experiments we invert this map numerically by means of the Newton method, iterated to convergence within machine accuracy.)

Figure 5 demonstrates the remarkable fact that for the limit process (4.1) with $\zeta = 10$ (which is highly underresolved), we observe convergence to the correct limit (2.8) in Fig. 6. (Note that the time steps here are 10 times larger than those used for the explicit schemes; this counterbalances

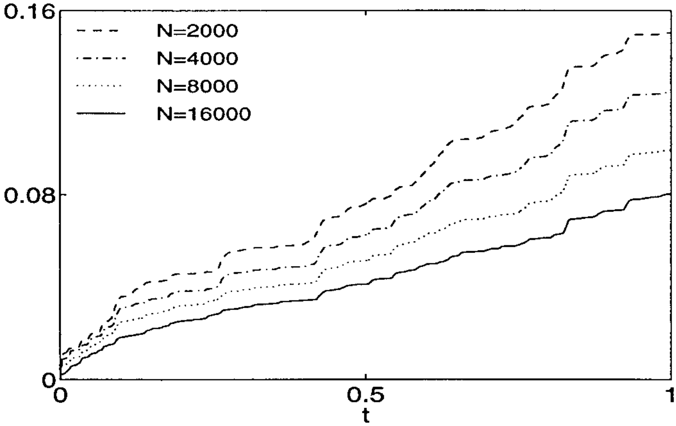

Fig. 6. $L^2(0, t)$ error curves in $\dot{q}(t)$ for backward Euler method (4.6) compared to $\dot{Q}(t)$ from the SDE (2.8).

the increased expense caused by the implicit nature of backward Euler.) Thus we conclude there is no direct relationship between symplectic methods and those which converge under the limit process (4.1). Different studies of the use of the backward Euler method in molecular dynamics may be found in ref. 20.

Despite these encouraging computational results concerning the backward Euler method, note that the experiments are performed over relatively short time intervals. We anticipate that over long time intervals the over-damping of backward Euler would impose severe limitations on the method. Because of the periodicity of K_N and Z_N given by (2.6), our limit problem as $N \to \infty$ has curious memory effects—for example, K_N becomes a *train* of delta functions and terms proportional to $\dot{q}(t-2k\pi)$ appear in the limit equation for any positive integer k such that $t > 2k\pi$. This gives rise to an interesting mathematical problem, but means that the study of long-time dynamics within the framework of this paper is somewhat of a curiousity and so we have not pursued it here.

5. NUMERICAL ANALYSIS

In this section we explain why some numerical methods (such as (4.3)) compute the correct macroscopic limit while others (such as (4.5)) do not. We show that a large family of numerical methods compute *a* macroscopic limit governed by a limiting SDE, but that this equation only co-incides with the correct macroscopic limit for certain parameters of the numerical method.

Note that the first two methods presented in section 4 are of the form:

$$\begin{aligned}
u_j^{n+1} &= u_j^n + v_j^n \, \Delta t - \alpha j^2 (u_j^n - q^n) \, \Delta t^2 \\
v_j^{n+1} &= v_j^n - j^2 (u_j^{n+1-\alpha} - q^{n+1-\alpha}) \, \Delta t, \\
q^{n+1} &= q^n + p^{n+\sigma_1} \, \Delta t, \\
p^{n+1} &= p^n - V'(q^{n+\sigma_2}) \, \Delta t + \gamma^2 \sum_{j=1}^{N} (u_j^{n+\theta} - q^{n+\phi}) \, \Delta t
\end{aligned} \tag{5.1}$$

where we define $\alpha, \sigma_i, \theta, \phi \in [0, 1]$ and for arbitrary sequence $\{W^n\}_{n \geqslant 0}$ and $\varepsilon \in [0, 1]$

$$W^{n+\varepsilon} = \varepsilon W^{n+1} + (1-\varepsilon) \, W^n.$$

In particular, the symplectic Euler method (4.3) has parameters

$$\alpha = 1, \qquad \theta = 0, \qquad \phi = 0, \qquad \sigma_1 = 1, \qquad \sigma_2 = 0 \tag{5.2}$$

whereas the perturbed method (4.5) has parameters

$$\alpha = 1, \qquad \theta = 1, \qquad \phi = 0, \qquad \sigma_1 = 1, \qquad \sigma_2 = 0 \tag{5.3}$$

Another symplectic Euler method can be obtained by choosing

$$\alpha = 0, \qquad \theta = 1, \qquad \phi = 1, \qquad \sigma_1 = 0, \qquad \sigma_2 = 1 \tag{5.4}$$

Our numerical experiments, including those given in Section 4, indicate that, under (4.1), the numerical method (5.1) approximates the correct SDE limit (2.8) only for certain combinations of the parameters α, θ and ϕ. In the following analysis we conjecture an SDE which (5.1) approximates under (4.1), explicitly stating the dependence of the SDE on the values of α, θ, ϕ and ζ. We thereby classify the methods which converge to the limiting SDE (2.8) and hence identify methods which recover the correct macroscopic behavior. For other values of α, θ and ϕ macroscopic behavior is computed but it is *incorrect*, being governed by an SDE different from (2.8)—namely (5.16). The analysis is purely formal and no proofs are given.

To facilitate the analysis we first combine the u_j^n and v_j^n terms in (5.1) to form an equation explicitly in terms of u_j^n, using (4.4) to determine the initial conditions:

$$\begin{aligned} &u_j^{n+1} - 2u_j^n + u_j^{n-1} + j^2\,\Delta t^2 (u_j^n - Q^n) = 0, \\ &u_j^0 = a_j, \qquad u_j^1 = a_j(1 - \alpha j^2\,\Delta t^2) + \alpha j^2\,\Delta t^2 q_0 \end{aligned} \tag{5.5}$$

Thus we observe that these methods solve for the homogeneous part of the heat bath in an energy-conserving manner for $j\,\Delta t \in [0, 2]$.[6]

We may solve the difference equation (5.5) by decomposing u_j^n into homogeneous and non-homogeneous components

$$u_j^n = W_j^n + \Lambda_j^n + q^n$$

These component sequences $\{W_j^n\}_{n \geq 0}$ and $\{\Lambda_j^n\}_{n \geq 0}$ satisfy the respective difference equations

$$\begin{aligned} W_j^{n+1} - 2W_j^n + W_j^{n-1} + j^2\,\Delta t^2 W_j^n &= 0, \\ W_j^0 = a_j, \qquad W_j^1 &= a_j(1 - \alpha j^2\,\Delta t^2) \\ \Lambda_j^{n+1} - 2\Lambda_j^n + \Lambda_j^{n-1} + j^2\,\Delta t^2 \Lambda_j^n + \delta^2 q^n &= 0, \\ \Lambda_j^0 = -q_0, \qquad \Lambda_j^1 &= -q_0(1 - \alpha j^2\,\Delta t^2) + (q_0 - q^1) \end{aligned} \tag{5.6}$$

[6] The energy of the numerical method is a small perturbation of the energy of the underlying harmonic oscillator.

with δ^2 denoting the second difference $\delta^2 q^n = q^{n+1} - 2q^n + q^{n-1}$. By standard techniques we solve for the explicit form of the homogeneous component W_j^n

$$W_j^n = a_j \frac{\cos(\phi_j n + \psi_j)}{\cos \psi_j}$$

where ϕ_j and ψ_j are determined by

$$\cos \phi_j = 1 - \frac{1}{2} j^2 \Delta t^2, \qquad \tan \psi_j = \frac{(\alpha - 1/2)\, j\, \Delta t}{\sqrt{1 - \frac{1}{4} j^2 \Delta t^2}}$$

and by variation of constants we obtain

$$\Lambda_j^n = -q_0 \frac{\cos(\phi_j n + \psi_j)}{\cos \psi_j} + (q_0 - q^1) \frac{\sin(\phi_j n)}{\sin \phi_j} - \sum_{m=1}^{n-1} \frac{\sin(\phi_j (n-m))}{\sin \phi_j} \delta^2 q^m$$

as the solution for the non-homogeneous component. To simplify the expression for Λ_j^n we apply summation by parts to obtain

$$\begin{aligned}(q_0 - q^1) \frac{\sin(\phi_j n)}{\sin \phi_j} &- \sum_{m=1}^{n-1} \frac{\sin(\phi_j (n-m))}{\sin \phi_j} \delta^2 q^m \\ &= -\sum_{m=0}^{n-1} \left[\frac{\sin(\phi_j (n-m)) - \sin(\phi_j (n-m-1))}{\sin \phi_j} \right] (q^{m+1} - q^m)\end{aligned}$$

giving the final form

$$\begin{aligned} u_j^n - q^n &= W_j^n + \Lambda_j^n \\ &= -\sum_{m=0}^{n-1} \left[\frac{\sin(\phi_j (n-m)) - \sin(\phi_j (n-m-1))}{\sin \phi_j} \right] (q^{m+1} - q^m) \\ &\quad + a_j \frac{\cos(\phi_j n + \psi_j)}{\cos \psi_j} - q_0 \frac{\cos(\phi_j n + \psi_j)}{\cos \psi_j} \end{aligned} \tag{5.7}$$

We rewrite the expression for p^{n+1} in (5.1) to take advantage of this derived expression for $u_j^n - q^n$

$$p^{n+1} = p^n - \Delta t\, V'(q^{n+\sigma_2}) + \Delta t\, \gamma^2 \sum_{j=1}^{N} (u_j^{n+\theta} - q^{n+\theta})$$
$$- \Delta t\, \gamma^2 \sum_{j=1}^{N} (\phi - \theta)(q^{n+1} - q^n)$$
$$= p^n - \Delta t\, V'(q^{n+\sigma_2}) + \Delta t\, \gamma^2 \sum_{j=1}^{N} (u_j^{n+\theta} - q^{n+\theta})$$
$$- \gamma^2 \zeta(\phi - \theta)(q^{n+1} - q^n)$$

Therefore summing (5.1) over n gives

$$q^n = q_0 + \Delta t \sum_{l=1}^{n-1} p^{l+\sigma_1},$$
$$p^n = p_0 - \Delta t \sum_{l=1}^{n-1} V'(q^{l+\sigma_2}) + \Delta t\, \gamma^2 \sum_{l=1}^{n-1} \sum_{j=1}^{N} (u_j^{l+\theta} - q^{l+\theta})$$
$$- \gamma^2 \zeta(\phi - \theta)\, \Delta t \sum_{l=0}^{n-1} \frac{q^{l+1} - q^l}{\Delta t} \tag{5.8}$$

Note that under the limiting process (4.1), certain terms in (5.8) appear to approximate known quanitites:

$$\Delta t \sum_{l=1}^{n-1} p^{l+\sigma_1} \approx \int_0^t p(s)\, ds$$
$$\Delta t \sum_{l=1}^{n-1} V'(q^{l+\sigma_2}) \approx \int_0^t V'(q(s))\, ds \tag{5.9}$$
$$\Delta t \sum_{l=1}^{n-1} \frac{q^{l+1} - q^l}{\Delta t} \approx \int_0^t p(s)\, ds$$

Thus the last term in (5.8) introduces an effective damping term with coefficient $\gamma^2 \zeta(\phi - \theta)$.

The double summation term in (5.8) also simplifies under the limiting process (4.1). Using the notation $\sum'$ to denote the weighted sum with weight θ on the first term, $(1-\theta)$ on the last term, and 1 otherwise, we reduce the double summation as follows

$$\Delta t\,\gamma^2 \sum_{l=1}^{n-1} \sum_{j=1}^{N} (u_j^{l+\theta} - q^{l+\theta})$$

$$= \Delta t\,\gamma^2 \sum_{l=0}^{n}{}' \sum_{j=1}^{N} (u_j^l - q^l)$$

$$= -\Delta t\,\gamma^2 \sum_{l=0}^{n}{}' \sum_{j=1}^{N} \sum_{m=0}^{l-1} \left[\frac{\sin(\phi_j(l-m)) - \sin(\phi_j(l-m-1))}{\sin \phi_j}\right] (q^{m+1} - q^m)$$

$$+ \Delta t\,\gamma^2 \sum_{l=0}^{n}{}' \sum_{j=1}^{N} a_j \frac{\cos(\phi_j n + \psi_j)}{\cos \psi_j} - \Delta t\,\gamma^2 q_0 \sum_{l=0}^{n}{}' \sum_{j=1}^{N} \frac{\cos(\phi_j n + \psi_j)}{\cos \psi_j} \tag{5.10}$$

Using the approximation

$$\Delta t \sum_{m=0}^{l-1} \left[\frac{\sin(\phi_j(l-m)) - \sin(\phi_j(l-m-1))}{\sin \phi_j}\right] \frac{q^{m+1} - q^m}{\Delta t}$$

$$\approx \int_0^{\tau} \cos(j(\tau - s))\, \dot{q}(s)\, ds$$

where $\tau = l\,\Delta t$, the triple sum in (5.10) thus appears to approximate the double integral

$$-\int_0^t \int_0^{\tau} K_{\mathrm{N}}(\tau - s)\, \dot{q}(s)\, ds\, d\tau \tag{5.11}$$

The convergence of the remaining terms in (5.10) however is more subtle. From Lemma A.1 in Appendix 2 (with $c_j \equiv 1$, $j \geqslant 1$, $c_0 = 0$, $f \equiv 0$) we see that the third term in (5.10) satisfies

$$-\Delta t\,\gamma^2 q_0 \sum_{l=0}^{n}{}' \sum_{j=1}^{N} \frac{\cos(\phi_j n + \psi_j)}{\cos \psi_j}$$

$$= -\gamma^2 q_0 \sum_{j=1}^{N} \xi_j \sin(\phi_j n) - (1 - \alpha - \theta)\, \gamma^2 q_0\, \Delta t \sum_{j=1}^{N} 2 \sin^2(\phi_j n/2)$$

$$\approx -q_0 \int_0^t \gamma^2 \sum_{j=1}^{N} \cos(js)\, ds - (1 - \alpha - \theta)\, \gamma^2 q_0\, \Delta t \sum_{j=1}^{N} 2 \sin^2(\phi_j n/2)$$

$$= -q_0 \int_0^t K_{\mathrm{N}}(s)\, ds - (1 - \alpha - \theta)\, \gamma^2 q_0\, \Delta t \sum_{j=1}^{N} [1 - \cos(\phi_j n)] \tag{5.12}$$

With the approximation $\phi_j n \approx jt$ we have

$$\Delta t^2 \left\| \sum_{j=1}^{N} \cos(\phi_j n) \right\|^2 \approx \Delta t^2 \left\| \sum_{j=1}^{N} \cos(jt) \right\|^2$$

$$= \Delta t^2 \sum_{j=1}^{N} \|\cos(jt)\|^2$$

$$= \mathcal{O}(\Delta t)$$

so that a jump of $-\gamma^2 \zeta\, q_0(1-\alpha-\theta)$ has been introduced in (5.12), to leading order in Δt. Lemma A.1 also applies to the second term in (5.10) (using $c_j \equiv a_j$, $j \geqslant 1$, $c_0 = 0$, $f \equiv 0$)

$$\begin{aligned}
&\Delta t\, \gamma^2 \sum_{l=0}^{n}{}' \sum_{j=1}^{N} a_j \frac{\cos(\phi_j n + \psi_j)}{\cos \psi_j} \\
&\quad = \gamma^2 \sum_{j=1}^{N} a_j \xi_j \sin(\phi_j n) + (1-\alpha-\theta)\, \gamma^2\, \Delta t \sum_{j=1}^{N} 2a_j \sin^2(\phi_j n/2) \\
&\quad \approx \int_0^t \gamma^2 a_j \sum_{j=1}^{N} \cos(js)\, ds + (1-\alpha-\theta)\, \gamma^2\, \Delta t \sum_{j=1}^{N} 2a_j \sin^2(\phi_j n/2) \\
&\quad = \int_0^t Z_{\mathbf{N}}(s)\, ds + (1-\alpha-\theta)\, \gamma^2\, \Delta t \sum_{j=1}^{N} a_j [1 - \cos(\phi_j n)]
\end{aligned} \tag{5.13}$$

the term proportional to $(1-\alpha-\theta)$ is $\mathcal{O}(\Delta t^{1/2})$ in expectation since the $\{a_j\}_{j=1}^{N}$ are IID Gaussian random variables, and thus it is negligible to leading order in Δt.

Collecting the expressions for (5.11)–(5.13), we see from (5.10) that the double summation in (5.8) approximates

$$\begin{aligned}
&\Delta t\, \gamma^2 \sum_{l=1}^{n-1} \sum_{j=1}^{N} (u_j^{l+\theta} - q^{l+\theta}) \\
&\quad \approx -\int_0^t \int_0^\tau K_{\mathbf{N}}(\tau - s)\, \dot{q}(s)\, ds\, d\tau + \int_0^t Z_{\mathbf{N}}(s)\, ds \\
&\qquad - q_0 \int_0^t K_{\mathbf{N}}(s)\, ds - \gamma^2 \zeta\, q_0(1-\alpha-\theta)
\end{aligned} \tag{5.14}$$

and also using (5.9), we deduce that (5.8) approximates

$$q(t) = q_0 + \int_0^t p(s)\, ds$$

$$p(t) = p_0 - \gamma^2\zeta\, q_0(1-\alpha-\theta) + \int_0^t V'(q(s))\, ds - \gamma^2\zeta(\phi-\theta)\int_0^t p(s)\, ds$$

$$-\int_0^t\int_0^\tau K_N(\tau-s)\,\dot{q}(s)\, ds\, d\tau - q_0\int_0^t K_N(s)\, ds + \int_0^t Z_N(s)\, ds$$

Hence we conjecture that under (4.1) the method (5.1) form approximates the differential equation

$$\begin{aligned} &\ddot{q} + \gamma^2\zeta(\phi-\theta)\,\dot{q} + V'(q) + \int_0^t K_N(t-s)\,\dot{q}(s) = -K_N(t)\,q_0 + Z_N(t) \\ &q(0) = q_0, \qquad \dot{q}(0) = p_0 - \gamma^2\zeta\, q_0(1-\alpha-\theta) \end{aligned} \tag{5.15}$$

and by the same methodology as in Section 3, as $N \to \infty$, (5.15) converges to the limiting SDE

$$\begin{aligned} &\ddot{Q} + \gamma^2\left\{\frac{\pi}{2} + \zeta(\phi-\theta)\right\}\dot{Q} + V'(Q) - \frac{\gamma^2}{2}Q = \dot{W}, \\ &Q(0) = q_0, \qquad \dot{Q}(0) = p_0 - \gamma^2 q_0\left\{\frac{\pi}{2} + \zeta(1-\alpha-\theta)\right\} \end{aligned} \tag{5.16}$$

We therefore conjecture that the numerical method (5.1) approximates the SDE (5.16) under the limiting process (4.1). Thus only for

$$\phi = \theta, \qquad \alpha = 1-\theta \tag{5.17}$$

will the method reproduce the correct macroscopic limiting behavior given by (2.8). Notice that this is achieved for both symplectic Euler methods (5.2) and (5.4) but not for the non-symplectic choice (5.3). This is consistent with the experiments in Section 4, which study (5.2) and (5.3). Note, however, that it is not necessary for the method to be symplectic in order that (5.17) hold, since (5.17) does not involve the parameters σ_1 and σ_2.

We illustrate that the formal argument leading to (5.16) is correct by performing a final experiment: we verify that the non-symplectic method (4.5) (equivalently (5.1), (5.3)) converges to the appropriate SDE of the form (5.16) under the limiting process (4.1). We first calculate an "exact" solution to (5.16) with values $\alpha = 1$, $\theta = 1$, $\phi = 0$ and $\zeta = 1$. This "exact"

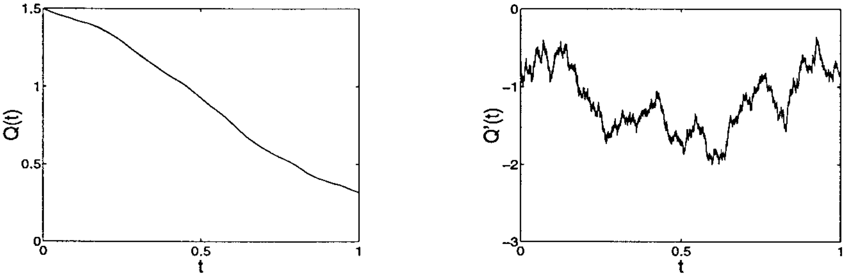

Fig. 7. Exact solutions Q and $\dot{Q}$ for the SDE (5.16) with $Q(0)=1.5$, $\dot{Q}(0)=0$ and parameter values $\alpha=1$, $\theta=1$, $\phi=0$.

solution is obtained by solving the following system of equations, analogous to (3.1), (3.2) but modified by damping and a shifted initial condition so that the limit $N \to \infty$ solves equation (5.16):

$$\ddot{q} + \gamma^2 \zeta(\phi - \theta)\, \dot{q} + V'(q) = \gamma^2 \sum_{j=1}^{N} (u_j - q),$$
$$\ddot{u_j} + j^2 (u_j - q) = 0, \tag{5.18}$$
$$q(0) = q_0, \qquad \dot{q}(0) = p_0 - \gamma^2 \zeta\, q_0 (1 - \alpha - \theta)$$

We take $N = 32{,}000$ and $N\,\Delta t = 10^{-3}$. These computed solutions for Q and $\dot{Q}$ are depicted in Fig. 7.

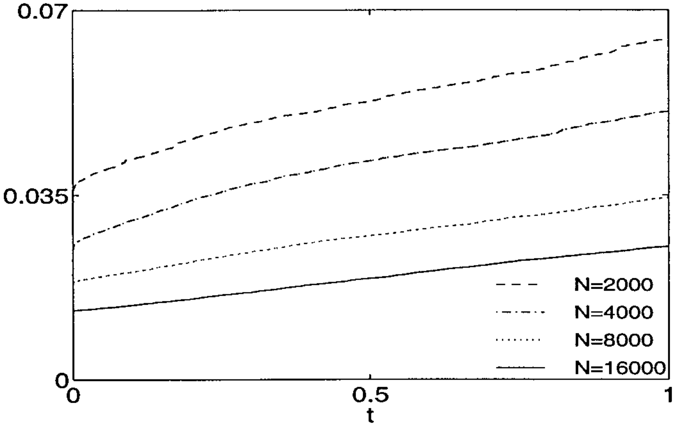

Fig. 8. $L^2(0, t)$ error curves in $\dot{q}(t)$ for non-symplectic scheme (4.5) compared to $\dot{Q}(t)$ from the SDE (5.16).

Comparing the solutions from (5.1), (5.3) to the "exact" solution of (5.16), we observe from the $L^2(0, t)$ error curves in Fig. 8 that the non-symplectic method (5.1), (5.3) does indeed converge to the solution of the appropriate *incorrect* SDE. For other methods with different values of α, θ and ϕ we also observe convergence to the appropriate SDE (5.16) under (4.1), suggesting our conjecture holds true.

6. SUMMARY AND DISCUSSION

We have analyzed a model of a heat bath, motivated by work of Ford and Kac;[9] this model is equivalent to several other heat bath models appearing in the statistical mechanics literature.[8] Our simple choice of parameters enables the proof of a sample path result relating the behavior of the observable to the solution of a Langevin equation.

Using this explicit Langevin limiting equation we have studied numerical methods for the heat bath in a computational regime with no resolution for fast scales—the stiff limit. Certain methods reproduce the correct Langevin equation while others compute an incorrect limit (still an SDE) with modified damping and shifted initial condition.

For many problems in computational molecular dynamics it is thought that an underlying stochastic process governs the behavior of the macroscopic quantities, but usually its form is not known analytically.[12] (If the limiting stochastic process *is* known exactly then it can be approximated directly by standard techniques.[13]) Furthermore in realistic problems no limit $N \to \infty$ is taken; we have simply introduced this limit artificially to enable a clear investigation of methods for Hamiltonian systems with broad frequency spectra. Thus the implication of our work for realistic problems, where an observable is computed by projecting the solution of a large system onto a low dimensional subspace, but for which no explicit effective stochastic process for the observable is known,[18, 19, 24] is unclear. However, at the very least, the work contained here suggests that similar studies for other problems in computational statistical mechanics may be valuable in understanding the sense in which simulations of large Hamiltonian systems in the stiff oscillatory regime may be considered accurate. A related, but different, perspective on underresolved dynamics may be found in refs. 4–6.

Previous work on the numerical simulation of stiff oscillatory systems has concentrated on Hamiltonian systems with the form

$$H(p, q) = \frac{1}{2} \|p\|^2 + V(q) + \frac{1}{\varepsilon^2} U(q), \qquad p, q \in \mathbb{R}^d \tag{6.1}$$

with governing equations of motion

$$\ddot{q} + \nabla V(q) + \frac{1}{\varepsilon^2} \nabla U(q) = 0 \tag{6.2}$$

If U achieves a global minimum on an m-dimensional manifold $\mathcal{M}$ which is strictly convex in its normal directions $N\mathcal{M}$, then the work of Rubin and Ungar[21] (and, by different methods, ref. 3) gives conditions under which q converges to a limit Q as $\varepsilon \to 0$, where Q solves

$$\ddot{Q} + \nabla V(Q) + \nabla V_a(Q) \in N_Q \mathcal{M} \tag{6.3}$$

Thus the limit is a differential algebraic equation with solution contrained to lie on $\mathcal{M}$. The additional potential V_a is non-zero when the initial velocities for (6.2) are not (close to) tangential to $\mathcal{M}$.

For such problems it is natural to ask which numerical methods, when applied to (6.2), accurately reproduce the limiting behviour given by (6.3), in the regime

$$\Delta t \to 0, \qquad \varepsilon \to 0, \qquad \Delta t = \varepsilon^{\alpha}, \qquad \alpha \in (0, 1] \tag{6.4}$$

(Note the analogy with our (4.1) since our fastest frequency is $\mathcal{O}(N)$; that in (6.2) is $\mathcal{O}(1/\varepsilon)$.) This convergence issue for stiff oscillatory problems is addressed very clearly for the case where $V_a \equiv 0$ in ref. 16 where, for example, the backward Euler method is shown to be effective under (6.4). The case where V_a is non-zero is harder as most methods under (6.4) tend to incorrectly approximate V_a by 0—experimental evidence of this behavior may be found in ref. 2.

Stability issues for the numerical solution of (6.2) (concerned with behavior for fixed $\Delta t \geqslant \mathcal{O}(\varepsilon)$ rather than under (6.4)) are investigated in ref. 10 and various papers by Schlick and co-workers.[17, 22, 23] In ref. 10 it is shown that coupling effects between fast and slow modes in Hamiltonian systems with symmetry can be incorrectly represented by certain numerical methods, such as the implicit midpoint rule, and similar analyses may be found in refs. 1 and 2; ref. 10 also show that an energy-momentum conserving integration has certain desirable features in this context. An alternative approach to the analysis of the instability of the implicit mid-point rule is presented in refs. 17, 22, and 23 where the instability is motivated as a resonance; symmetry considerations are not invoked. Various fixes are suggested to inhibit the resonances or delay their occurence to larger Δt.

A major drawback of the work just outlined concerning stability is that it fails to address the sense in which stable calculation of stiff (oscillatory) Hamiltonian systems are *accurate*—except through behavior of the energy. This issue is addressed to some extent by Ascher and Reich[(2)] who study, for stable schemes with large time steps, the behavior of certain slowly varying quantities (adiabatic invariants); however it appears hard to prove anything about approximations of slowly varying quantities in generality by their techniques.

We have chosen a large Hamiltonian system related to, but somewhat different from, (6.2) in which we *are* able to address the question of the interaction between stability considerations (roughly, choosing time steps to prevent blow-up through fast frequencies, but neglecting their accuracy) and accuracy considerations (roughly, asking that slowly evolving quantities are computed accurately). The framework in which we do this is to consider the dimension of the system going to infinity as we are then able to establish a theorem concerning the evolution of slow variables through an SDE. The resulting model may seem contrived from the viewpoint of real molecular dynamics simulations but it does allow us to address carefully a question of real importance concerning the accuracy of simulations for stiff Hamiltonian systems. In the future it would be desirable to extend these ideas to other Hamiltonian systems where slow variables are governed by random differential equations, but where the underlying system is of finite dimension and close connection with (6.2) is made.

APPENDIX 1

Proof of Lemma 3.2. We define

$$\hat{R}_{\mathrm{N,\,M}}(t) := \gamma^2 \sum_{j=N+1}^{M} \frac{1}{j} \sin(jt)$$

Noting that, as $M \to \infty$ for fixed N,

$$\left\| \int_0^t \hat{R}_{\mathrm{N,\,M}}(t-s)\, A(s)\, ds \right\|^2 \to \left\| \int_0^t \bar{R}_{\mathrm{N}}(t-s)\, A(s)\, ds \right\|^2$$

for any $A \in L^2(0, \pi)$, it thus suffices to obtain bounds on the two terms in Lemma 3.2 with $\hat{R}_{\mathrm{N,\,M}}$ replacing $\bar{R}_{\mathrm{N}}$.

It will be useful to define

$$a_{k,\,j}(t) = \frac{1}{j} \int_0^t \sin[\,j(t-s)]\cos(ks)\, ds$$

Integration shows that

$$a_{k,j}(t) = \frac{\cos(kt) - \cos(jt)}{j^2 - k^2}$$

We let $\sum^*$ denote summation with weight $\frac{1}{2}$ on the first term. A straightforward calculation shows that

$$\int_0^t \hat{R}_{\mathbf{N},\mathbf{M}}(t-s)\left[\frac{\gamma^2}{2} + K_{\mathbf{N}}(s)\right] ds = \gamma^4 \sum_{j=N+1}^{M} \left(\sum_{k=0}^{N}{}^{*} a_{k,j}(t) \right)$$

Thus

$$\left\| \int_0^t \hat{R}_{\mathbf{N},\mathbf{M}}(t-s)\left[\frac{\gamma^2}{2} + K_{\mathbf{N}}(s)\right] ds \right\|^2 = \gamma^8 \sum_{i,j=N+1}^{M} \sum_{k,l=0}^{N}{}^{*} \int_0^{\pi} a_{k,j}(t)\, a_{l,i}(t)\, dt$$

But, using $k, l < i, j$ we obtain

$$\int_0^{\pi} a_{k,j}(t)\, a_{l,i}(t)\, dt = \pi \frac{\delta_{kl}}{2(j^2-k^2)(i^2-k^2)} + \pi \frac{\delta_{ij}}{2(j^2-k^2)(j^2-l^2)}$$

Hence

$$\left\| \int_0^t \hat{R}_{\mathbf{N},\mathbf{M}}(t-s)\left[\frac{\gamma^2}{2} + K_{\mathbf{N}}(s)\right] ds \right\|^2$$

$$= \frac{\pi\gamma^8}{2} \sum_{i,j=N+1}^{M} \sum_{k=0}^{N}{}^{*} \frac{1}{(j^2-k^2)(i^2-k^2)} + \frac{\pi\gamma^8}{2} \sum_{j=N+1}^{M} \sum_{k,l=0}^{N}{}^{*} \frac{1}{(j^2-k^2)(j^2-l^2)}$$

Thus

$$\left\| \int_0^t \hat{R}_{\mathbf{N},\mathbf{M}}(t-s)\left[\frac{\gamma^2}{2} + K_{\mathbf{N}}(s)\right] ds \right\|^2$$

$$= \frac{\pi\gamma^8}{2} \sum_{k=0}^{N} \left(\sum_{j=N+1}^{M} \frac{1}{j^2-k^2} \right)^2 + \frac{\pi\gamma^8}{2} \sum_{j=N+1}^{M} \left(\sum_{k=0}^{N}{}^{*} \frac{1}{j^2-k^2} \right)^2 \qquad \text{(A.1.1)}$$

Now we consider the second integral which requires bounding and show that it also satisfies a bound like (A.1.1). Clearly

$$\int_0^t \hat{R}_{\mathbf{N},\mathbf{M}}(t-s)\, Z_{\mathbf{N}}(s)\, ds = \frac{\gamma^3}{\sqrt{\beta}} \sum_{j=N+1}^{M} \sum_{k=1}^{N} \mu_k\, a_{k,j}(t)$$

Hence

$$\mathbb{E}\left\|\int_0^t \hat{R}_{\mathbf{N},\mathbf{M}}(t-s)\,Z_{\mathbf{N}}(s)\,ds\right\|^2 = \frac{\gamma^6}{\beta}\sum_{i,\,j=N+1}^{M}\;\sum_{k,\,l=1}^{N}\int_0^{\pi} a_{k,\,j}(t)\,a_{l,\,i}(t)\,\delta_{kl}\,dt$$

so that

$$\mathbb{E}\left\|\int_0^t \hat{R}_{\mathbf{N},\mathbf{M}}(t-s)\,Z_{\mathbf{N}}(s)\,ds\right\|^2 = \frac{\gamma^6}{\beta}\sum_{i,\,j=N+1}^{M}\;\sum_{k=1}^{N}\int_0^{\pi} a_{k,\,j}(t)\,a_{k,\,i}(t)\,dt$$

Now, since $i,\ j>k$,

$$\begin{aligned}\int_0^{\pi} a_{k,\,j}(t)\,a_{k,\,i}(t)\,dt &= \int_0^{\pi}\left[\frac{\cos(kt)-\cos(jt)}{j^2-k^2}\right]\left[\frac{\cos(kt)-\cos(it)}{i^2-k^2}\right]dt\\ &= \frac{\pi}{2(j^2-k^2)(i^2-k^2)}+\frac{\pi\delta_{ij}}{2(j^2-k^2)^2}\end{aligned}$$

Thus

$$\begin{aligned}&\mathbb{E}\left\|\int_0^t \hat{R}_{\mathbf{N},\mathbf{M}}(t-s)\,Z_{\mathbf{N}}(s)\,ds\right\|^2\\ &\quad=\frac{\pi\gamma^6}{2\beta}\sum_{i,\,j=N+1}^{M}\;\sum_{k=1}^{N}\left\{\frac{1}{(j^2-k^2)(i^2-k^2)}+\frac{\delta_{ij}}{(j^2-k^2)^2}\right\}\\ &\quad=\frac{\pi\gamma^6}{2\beta}\left[\sum_{k=1}^{N}\left(\sum_{j=N+1}^{M}\frac{1}{j^2-k^2}\right)^2+\sum_{j=N+1}^{M}\;\sum_{k=1}^{N}\frac{1}{(j^2-k^2)^2}\right]\\ &\quad\leqslant\frac{\pi\gamma^6}{2\beta}\left[\sum_{k=0}^{N}{}^{*}\left(\sum_{j=N+1}^{M}\frac{1}{j^2-k^2}\right)^2+\sum_{j=N+1}^{M}\left(\sum_{k=0}^{N}{}^{*}\frac{1}{j^2-k^2}\right)^2\right]\end{aligned}$$

In summary we have shown that both terms which we need to estimate are bounded by an expression of the form

$$C\left[\sum_{k=0}^{N}{}^{*}\left(\sum_{j=N+1}^{\infty}\frac{1}{j^2-k^2}\right)^2+\sum_{j=N+1}^{\infty}\left(\sum_{k=0}^{N}{}^{*}\frac{1}{j^2-k^2}\right)^2\right]$$

We now bound both terms in this expression. The first, I, may be usefully re-written as follows:

$$\begin{aligned} I &= \sum_{k=0}^{N}{}^{*}\left(\sum_{j=N+1}^{\infty}\frac{1}{j^2-k^2}\right)^2 \\ &\leqslant \sum_{k=1}^{N}\left(\frac{1}{2k}\sum_{j=N+1}^{\infty}\left[\frac{1}{j-k}-\frac{1}{j+k}\right]\right)^2+\frac{1}{2}\left(\sum_{j=N+1}^{\infty}\frac{1}{j^2}\right) \\ &\leqslant \sum_{k=1}^{N}\left(\frac{1}{2k}\sum_{l=N+1-k}^{N+k}\frac{1}{l}\right)^2+\frac{1}{2N} \\ &= \sum_{k=1}^{N} a_k^2+\frac{1}{2N} \end{aligned}$$

where

$$a_k := \frac{1}{2k}\sum_{l=N+1-k}^{N+k}\frac{1}{l}$$

Hence

$$a_{k+1} = \frac{1}{k+1}\left(ka_k+\frac{1}{2(N-k)}+\frac{1}{2(N+k+1)}\right)$$

so that

$$a_{k+1} \leqslant a_k+\frac{2N+1}{2(k+1)(N-k)(N+k+1)}$$

Thus $a_1 \leqslant 1/N$ and

$$a_{k+1} \leqslant a_k+\frac{1}{(k+1)(N-k)} = a_k+\frac{1}{N+1}\left(\frac{1}{k+1}+\frac{1}{N-k}\right)$$

Consequently

$$a_k \leqslant a_1+\frac{1}{N+1}\sum_{l=1}^{k-1}\left(\frac{1}{l+1}+\frac{1}{N-l}\right) \leqslant \frac{2}{N+1}+\frac{2}{N+1}\sum_{l=1}^{N-1}\frac{1}{l}$$

Now

$$\sum_{l=1}^{N}\frac{1}{l} \leqslant 2\ln(N+1) \tag{A.1.2}$$

Thus, using (A.1.2),

$$a_k \leqslant 2\,\frac{(1+2\ln N)}{N+1}$$

Thus

$$\begin{aligned} I &\leqslant \sum_{k=0}^{N} \frac{4(1+2\ln N)^2}{(N+1)^2} \\ &\leqslant 4\,\frac{(1+2\ln N)^2}{N+1} \\ &= \mathcal{O}\left(\frac{(\ln N)^2}{N}\right) \end{aligned}$$

The required result follows if we can estimate the second term, *II*, similarly. This is straightforward:

$$\begin{aligned} II &= \sum_{j=N+1}^{\infty} \left(\sum_{k=0}^{N}{}^{*}\, \frac{1}{j^2-k^2}\right)^2 \\ &= \sum_{j=N+1}^{\infty} \left[\frac{1}{2j^2} + \sum_{k=1}^{N} \left(\frac{1}{2j(j-k)} + \frac{1}{2j(j+k)}\right)\right]^2 \\ &\leqslant \sum_{j=N+1}^{\infty} \frac{1}{4j^2}\left[\frac{1}{j} + \sum_{k=1}^{N} \frac{2}{j-k}\right]^2 \\ &\leqslant \sum_{j=N+1}^{\infty} \frac{1}{4j^2}\left[\frac{2}{N+1} + \sum_{k=1}^{N} \frac{2}{N+1-k}\right]^2 \\ &\leqslant \sum_{j=N+1}^{\infty} \frac{1}{4j^2}\, 16(\ln(N+2))^2 \\ &= \mathcal{O}\left(\frac{(\ln N)^2}{N}\right) \quad \blacksquare \end{aligned}$$

APPENDIX 2

To motivate the introduction of the extraneous terms in (5.12), (5.13) by the method (5.1) form we examine a simpler model problem which isolates this behavior.

Consider the equations

$$\ddot{u}_j + j^2 u_j = 0, \qquad u_j(0) = c_j, \qquad \dot{u}_j(0) = 0, \qquad j = 0,..., N \tag{A.2.1}$$

and

$$\dot{z} = f(z) + H_{\mathbf{N}}(t), \qquad z(0) = z_0 \tag{A.2.2}$$

where

$$H_{\mathbf{N}}(t) := \sum_{j=0}^{N} u_j(t)$$

Note that for the choice of

$$c_0 = 0, \qquad c_j = \gamma^2, \qquad j = 1,..., N$$

then

$$H_{\mathbf{N}}(t) = K_{\mathbf{N}}(t)$$

whereas for the values

$$c_0 = 0, \qquad c_j = \frac{\gamma}{\sqrt{\beta}}\, \mu_j, \qquad j = 1,..., N$$

with $\{\mu_j\}_{j=1}^{N}$ $\mathcal{N}(0, 1)$, IID random variables,

$$H_{\mathbf{N}}(t) = Z_{\mathbf{N}}(t)$$

We solve (A.2.1) by the following paramaterized energy-conserving methods analogous to (5.5)

$$u_j^{n+1} - 2u_j^n + u_j^{n-1} + j^2\, \Delta t^2 u_j^n = 0, \qquad u_j^0 = c_j, \qquad u_j^1 = c_j[1 - \alpha j^2\, \Delta t^2] \tag{A.2.3}$$

for $\alpha \in [0, 1]$ and solve (A.2.2) by the θ-method (for $t^n := n\,\Delta t$)

$$Z^{n+1} - Z^n = \Delta t\,[\theta f(Z^{n+1}) + (1-\theta)\, f(Z^n)] + \Delta t\,[\theta H_{\mathbf{N}}^{\Delta t}(t^{n+1}) + (1-\theta)\, H_{\mathbf{N}}^{\Delta t}(t^n)]$$

where

$$H_{\mathrm{N}}^{\Delta t}(t^n) = \sum_{j=0}^{N} u_j^n$$

and with $Z(0) = z_0$. The numerical solution $\{Z^n\}_{n \geqslant 0}$ from this method has the following form:

Lemma A.1. The sequence $\{Z^n\}_{n \geqslant 0}$ generated by (A.2.4) satisfies

$$Z^n = z_0 + \Delta t \sum_{m=0}^{n}{}' f(Z^m) + (n\,\Delta t)\, c_0 + \sum_{j=1}^{N} c_j \xi_j \sin(\phi_j n)$$
$$+ (1-\theta-\alpha)\,\Delta t \sum_{j=1}^{N} 2c_j \sin^2(\phi_j n/2)$$

where $\sum_{m=0}^{\prime n}$ denotes a sum with weight $(1-\theta)$ on $m=0$, θ on $m=n$, and 1 otherwise. Furthermore ϕ_j and ξ_j are given by

$$\cos\phi_j = 1 - \tfrac{1}{2} j^2\, \Delta t^2$$

and

$$\xi_j = \frac{\sqrt{1-\frac{1}{4} j^2\, \Delta t^2}}{j} + \frac{(\alpha - \frac{1}{2})(\frac{1}{2}-\theta)\, j\, \Delta t^2}{\sqrt{1-\frac{1}{4} j^2\, \Delta t^2}}$$

Note that the exact solution at $t^n = n\,\Delta t$ satisfies

$$z(n\,\Delta t) = z_0 + \int_0^{n\,\Delta t} f(z(s))\, ds + (n\,\Delta t)\, c_0 + \sum_{j=1}^{N} c_j\, \frac{\sin(jn\Delta t)}{j}$$

Thus the numerical method introduces an extra $\mathcal{O}(\theta+\alpha-1)$ jump term into the solution.

Proof. Summing (A.2.4) over n gives

$$Z^n = z_0 + \Delta t \sum_{m=0}^{n}{}' f(Z^m) + \Delta t \sum_{m=0}^{n}{}' H_{\mathrm{N}}^{\Delta t}(t^m)$$

so to complete the proof we only need show

$$h_{\mathrm{N}}^{\Delta t}(t^n) := \Delta t \sum_{m=0}^{n}{}' H_{\mathrm{N}}^{\Delta t}(t^m)$$
$$= (n\,\Delta t)\, c_0 + \sum_{j=1}^{N} c_j \xi_j \sin(\phi_j n) + (1-\theta-\alpha)\,\Delta t \sum_{j=1}^{N} 2c_j \sin^2(\phi_j n/2)$$

The general form of the solution to the difference equation (A.2.3) is

$$u_j^n = e^{i\phi_j n}$$

and through standard manipulation we have

$$\cos\phi_j = 1 - \tfrac{1}{2} j^2\,\Delta t^2$$
$$\sin\phi_j = j\,\Delta t\,\sqrt{1 - \tfrac{1}{4} j^2\,\Delta t^2}$$

To satisfy the initial conditions, the solution is given by

$$u_j^n = c_j\,\frac{\cos(\phi_j n + \psi_j)}{\cos\psi_j}$$

where ψ_j satisfies

$$\tan\psi_j = \frac{(\alpha - \frac{1}{2})\,j\,\Delta t}{\sqrt{1 - \frac{1}{4} j^2\,\Delta t^2}}$$

Thus

$$\begin{aligned} h_{\mathrm{N}}^{\Delta t}(t^n) &= \Delta t \sum_{m=0}^{n}{}' \sum_{j=0}^{N} c_j\,\frac{\cos(\phi_j m + \psi_j)}{\cos\psi_j} \\ &= (n\,\Delta t)\,c_0 + \Delta t \sum_{j=1}^{N} c_j \sum_{m=0}^{n}{}' \frac{\cos(\phi_j m + \psi_j)}{\cos\psi_j} \\ &= (n\,\Delta t)\,c_0 + \Delta t \sum_{j=1}^{N} c_j \left(\sum_{m=0}^{n-1} \frac{\cos(\phi_j m + \psi_j)}{\cos\psi_j} + \theta\left[\frac{\cos(\phi_j n + \psi_j)}{\cos\psi_j} - 1\right]\right) \end{aligned}$$

From Eq. 1.341(3) in ref. 11,

$$\begin{aligned} h_{\mathrm{N}}^{\Delta t}(t^n) = \Delta t \sum_{j=1}^{N} c_j &\left\{ \frac{\cos(\psi_j + ((n-1)/2)\,\phi_j)\,\sin(\phi_j n/2)}{\cos\psi_j\,\sin(\phi_j/2)} \right. \\ &\left. + \theta\left[\frac{\cos(\phi_j n + \psi_j)}{\cos\psi_j} - 1\right]\right\} + (n\,\Delta t)\,c_0 \end{aligned}$$

and by expansion

$$\begin{aligned} \cos\left(\psi_j + \left(\frac{n-1}{2}\right)\phi_j\right) = \cos\left(\frac{\phi_j n}{2}\right)&\left[\cos\psi_j \cos\frac{\phi_j}{2} + \sin\psi_j \sin\frac{\phi_j}{2}\right] \\ - \sin\left(\frac{\phi_j n}{2}\right)&\left[\sin\psi_j \cos\frac{\phi_j}{2} - \cos\psi_j \sin\frac{\phi_j}{2}\right] \end{aligned}$$

This gives

$$\frac{\cos(\psi_j + ((n-1)/2)\,\phi_j)\sin(\phi_j n/2)}{\cos\psi_j \sin(\phi_j/2)} = \frac{1}{2}\frac{\sin(\phi_j n)}{\tan(\phi_j/2)} + \frac{1}{2}\sin(\phi_j n)\tan\psi_j + \left(\frac{\cos(\phi_j n)-1}{2}\right)\left(\frac{\tan\psi_j}{\tan(\phi_j/2)} - 1\right)$$

Now using the identities

$$\frac{\tan\psi_j}{\tan(\phi_j/2)} = 2\alpha - 1, \qquad \tan^2(\phi_j/2) = \frac{j^2\,\Delta t^2}{4 - j^2\,\Delta t^2}$$

and the known expression of $\tan\psi_j$, we conclude with

$$\begin{aligned} h_{\mathrm{N}}^{\Delta t}(t^n) &= (n\,\Delta t)\,c_0 + \Delta t \sum_{j=1}^{N} c_j \left\{\frac{1}{2}\frac{\sin(\phi_j n)}{\tan(\phi_j/2)} + \left(\frac{1}{2} - \theta\right)\sin(\phi_j n)\tan\psi_j\right\} \\ &\quad - (1-\alpha-\theta)\,\Delta t \sum_{j=1}^{N} c_j[\cos(\phi_j n) - 1] \\ &= (n\,\Delta t)\,c_0 + \sum_{j=1}^{N} c_j \xi_j \sin(\phi_j n) \\ &\quad + (1-\alpha-\theta)\,\Delta t \sum_{j=1}^{N} 2c_j \sin^2(\phi_j n/2) \quad \blacksquare \end{aligned}$$

ACKNOWLEDGMENTS

The work of A.M.S. was supported by the National Science Foundation under Grant DMS-95-0487 and by the EPSRC, U.K. The work of J.O.W. was supported by a Department of Defense National Defense Science and Engineering Graduate Fellowship Program.

REFERENCES

1. U. Ascher and S. Reich, On some difficulties in integrating highly oscillatory Hamiltonian systems, *Proc. Alg. for Macromolecular Modelling*, 1997.
2. U. Ascher and S. Reich, The midpoint scheme and variants for Hamiltonian systems: Advantages and pitfalls, *SIAM J. Sci. Comp.*, to appear.
3. F. Bornemann and Schütte, Homogenization of Hamiltonian systems with a strong constraining potential, *Physica D* **102**:57–77 (1997).
4. A. J. Chorin, A. Kast, and R. Kupferman, On the prediction of large-scale dynamics using underresolved computations. Submitted to *AMS Contemporary Mathematics*, 1998.

5. A. J. Chorin, A. Kast, and R. Kupferman, Unresolved computation and optimal predictions, *Comm. Pure Appl. Math.*, to appear.
6. A. J. Chorin, A. Kast, and R. Kupferman, Optimal prediction of underresolved dynamics, *Proc. Nat. Acad. Sci. USA* **95**:4094–4098 (1998).
7. B. Cano, A. Stuart, E. Süli, and J. Warren, Stiff oscillatory systems, delta jumps and white noise, Technical Report SCCM-99-01, http://www-sccm.stanford.edu/pub/sccm/sccm-99-01.ps.gz.
8. G. W. Ford, J. T. Lewis, and R. F. O'Connell, Quantum Langevin equation, *Phys. Rev. A* **37**:4419–4428 (1988).
9. G. W. Ford and M. Kac, On the quantum Langevin equation, *J. Stat. Phys.* **46**:803–810 (1987).
10. O. Gonzalez and J. C. Simo, On the stability of symplectic and energy-momentum algorithms for nonlinear Hamiltonian systems with symmetry, *Comp. Meth. Appl. Mech. Eng.* **134**:197–222 (1996).
11. I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, New York, 1965).
12. H. Grubmüller and P. Tavan, Molecular dynamics of conformational substates for a simplified protein model, *J. Chem. Phys.* **101**:5047–5057 (1994).
13. J. Honerkamp, *Stochastic Dynamical Systems: Concepts Numerical Methods, Data Analysis* (VCH Publishers, New York, 1994).
14. V. Jakšić and C.-A. Pillet, Ergodic properties of the Langevin equation, *Lett. Math. Phys.* **41**:49–57 (1997).
15. N. V. Krylov, *Introduction to the Theory of Diffusion Processes*, AMS Translations of Monographs, Volume 142 (1994).
16. C. Lubich, Integration of stiff mechanical systems by Runge–Kutta methods, *ZAMP* **44**:1022–1053 (1993).
17. M. Mandziuk and T. Schlick, Resonance in the dynamics of chemical systems simulated by the implicit midpoint scheme, *Chem. Phys. Lett.* **237**:525–535 (1995).
18. H. Mori, Transport, collective motion, and Brownian motion, *Prog. Theor. Phys.* **33**:423–455 (1964).
19. S. Nordholm and R. Zwanzig, A systematic derivation of generalized Brownian motion theory, *J. Stat. Phys.* **13**:347–371 (1975).
20. C. S. Peskin and T. Schlick, Molecular dynamics by the backward Euler method, *Comm. Pure Appl. Math.* **XLII**:1001–1031 (1989).
21. H. Rubin and P. Ungar, Motion under a strong constraining force, *Comm. Pure. Appl. Math Appl. Math.* **X**:65–87 (1957).
22. T. Schlick, M. Mandziuk, R. Skeel and K. Srinivas, Nonlinear resonance artifacts in molecular dynamics simulations, *J. Comp. Phys.* **140**:1–29 (1998).
23. R. D. Skeel, G. Zhang, and T. Schlick, A family of symplectic integrators: Stability, accuracy and molecular dynamics applications, *SIAM J. Sci. Comp.* **18**:203–222 (1997).
24. R. Zwanzig, Ensemble method in the theory of irreversibility, *J. Chem. Phys.* **33**:1339–1341 (1960).