The Kramers equation simulation algorithm:

I. Operator analysis

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Abstract

Using an operatorial formalism, we study the Kramers equation and its applications to numerical simulations. We obtain classes of algorithms which may be made precise at every desired order in the time step $\epsilon$ and with a set of free parameters which can be used to reduce autocorrelations. We show that it is possible to use a global Metropolis test to restore Detailed Balance.

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I. INTRODUCTION

Quantum field theories can be numerically simulated on a lattice to obtain non perturbative informations. A definite continuum limit not always exists, but for many interesting theories asymptotic freedom allows for the extraction of continuum physics from the lattice. The algorithmic problem of the Monte Carlo approach amounts to generate many statistically independent configurations of the fields. These configurations must be distributed according to a definite weight which depends on the specific action of the model. We have a great freedom in building such a procedure. A possible strategy is based on the idea of obtaining the final target distribution via a diffusion process in the configuration space which gives asymptotically infinite configurations properly distributed. A numerical simulation of the above continuous diffusion process leads naturally to approximated schemes for the generation of the equilibrium ensemble. Indeed, solving the diffusion process is like integrating a differential equation and some kind of extrapolation in the integration step must be done at the end to get the exact results. On the other hand, exact algorithms may be obtained with the introduction of a Metropolis test, namely a global recall of the action that we are simulating. Depending on the problem under study one of the two choices may be preferable. In this work we show how one can generalize the simplest Langevin process

\[ q_{n+1} = q_n + \Delta_{\alpha_n} e_{\alpha_n} \] where \( \{e_{\alpha}\} \) identifies all the possible directions on the lattice and \( \Delta_{\alpha} \) is the space step in the \( \alpha \)-th direction. The relevant direction \( \alpha \) is chosen with a definite space-dependent probability \( P_{\alpha} \) such that as \( t \to +\infty \) with \( \Delta_{\alpha} \to 0 \) a definite distribution for the configurations in \( \{q_n\} \) is obtained.

\[ ^1 \text{In [1] we have studied a different implementation of the diffusion process. A diffusive process can be realized on a discrete space-time. The correct diffusion equation in the continuum is obtained only at the end with a careful limit in both the spatial and temporal steps. Ref. [1] showed the applicability and power of this method in the framework of the First-Exit-Mean-Time problems. Space becomes discrete and at every sweep the degrees of freedom } q_n \text{ are modified to } q_{n+1} = q_n + \Delta_{\alpha_n} e_{\alpha_n} \text{ where } \{e_{\alpha}\} \text{ identifies all the possible directions on the lattice and } \Delta_{\alpha} \text{ is the space step in the } \alpha \text{-th direction. The relevant direction } \alpha \text{ is chosen with a definite space-dependent probability } P_{\alpha} \text{ such that as } t \to +\infty \text{ with } \Delta_{\alpha} \to 0 \text{ a definite distribution for the configurations in } \{q_n\} \text{ is obtained.} \]
to more complicated and efficient schemes. We also show which global correction must be performed in order to restore the Detailed Balance condition.

In Sec. I we recall the basic ideas of the Monte Carlo approach to numerical simulations. In Sec. II we introduce formalism and notation discussing the Langevin and the Horowitz algorithms. In Sec. III we show their natural extensions and discuss in Sec. IV their autocorrelations in the continuum. In Sec. V we show exact versions of these schemes. Some comment are collected in Sec. VII on the relations with existing algorithms. Finally, Sec. VIII is devoted to the conclusions. In Appendix A we illustrate the symplectic methods for the integration of the equations of motion. Finally, in Appendix B and C some technical notes are collected.

II. MONTE CARLO SIMULATIONS

Let us consider $R^n$ flat space with Euclidean measure. Given the degrees of freedom $\{q\}$ and the action $S(q)$ (a scalar function of the $q$) we want to generate efficiently samples of statistically independent configurations distributed according to the weight

$$P(q) = e^{-\beta S(q)},$$

(2.1)

where $\beta$ is the inverse temperature of the system under study. The strategy of Monte Carlo simulations is to start from a random initial configuration and to evolve it along a discrete Markov chain determined by a given transition probability

$$P(q' \rightarrow q'') \int P(q' \rightarrow q'') \ dq'' = 1$$

(2.2)

which is the probability of making a transition from $q'$ to $q''$. We know [3] that if the above Markov chain is irreducible and a stationary state $W(q)$ exists satisfying the stationarity condition

$$\int W(q')P(q' \rightarrow q'') \ dq' = W(q''),$$

(2.3)
then the process will converge to $W(q)$. A sufficient but not necessary condition to satisfy Eq. (2.3) is the stronger *Detailed Balance* condition

$$W(q') P(q' \to q'') = W(q'') P(q'' \to q').$$

(2.4)

More generally, a powerful trick is to make the action depend on some auxiliary variables $\xi$ which diffuse together with the $q$ and satisfy

$$S(q) \rightarrow \tilde{S}(q, \xi) \quad \text{such that} \quad \int d\xi e^{\tilde{S}(q, \xi)} \sim e^{S(q)}.$$  

(2.5)

Averages of functionals independent of $\xi$ are equal to those obtained with $S(q)$. Detailed Balance will be encoded by a generalized Eq. (2.3) of the form

$$W(q', \xi) P(q', \xi \to q'', \xi'') = W(q'', T \xi'') P(q'', T \xi'' \to q', T \xi'),$$

(2.6)

where $T \xi$ is the transformed of $\xi$ under time reversal.

Choosing the best transition probability depends on the nature of the problem under study and on which kind of measurements one is interested in. Moreover, for practical implementations, it is relevant to know the specific architecture of the machine which one will use. As we have explained in the introduction, a natural idea is to take advantage of a continuum dynamics towards equilibrium. This leads us to consider the Fokker-Planck diffusion equation [4], the Langevin algorithm and its generalizations.

**III. FOKKER-PLANCK EVOLUTION**

The standard Fokker-Planck equation for the diffusion in $R^n$ may be written

$$-\frac{\partial P}{\partial t} = HP,$$

(3.1)

where the evolution kernel for the time dependent probability distribution $P(q,t)$ is

$$H = \frac{1}{\beta} \Pi^2 + i \Pi F(q) \quad \Pi = -i \frac{\partial}{\partial q}$$

(3.2)

and $F(q)$ is the driving force which we assume derived from a potential
\[ F(q) = -i\Pi S(q). \] (3.3)

Eq. (3.1) describes relaxation towards the static distribution

\[ W(q) = e^{-\beta S(q)}. \] (3.4)

This can be shown in the continuum evolution as follows \[5\]. Consider the scalar product (we restrict ourselves to real functions)

\[(f, h) = \int (dq)W \cdot f(q)h(q) \quad (dq)_W = dq \quad [W(q)]^{-1}, \] (3.5)

then we have

\[(f, Hf) = \int (dq)_W f(q)\Pi \left\{ \frac{1}{\beta}\Pi + iF(q) \right\} f(q) = -\frac{1}{\beta} \int dqW(q) \left\{ \Pi f(q) [W(q)]^{-1} \right\}^2. \] (3.6)

\[ W(q) \] is an eigenstate of \( H \) with zero eigenvalue. From the above equation it follows that if \( Hf = 0 \) then \( f \sim W(q) \) whence \( W(q) \) is the unique stable mode. Moreover from Eq. (3.6) we deduce that all the other eigenvalues of \( H \) are negative. Therefore, by expanding a generic solution \( u(q, t) \) of Eq. (3.1) in a basis of \( H \) eigenvectors we show that \( u \to W \) as \( t \to +\infty \).

Consider now the Markov chain defined by the following real transition probability

\[ P(q' \to q'') = \langle q'' | \exp (-\epsilon H) | q' \rangle \overset{def}{=} \langle q'' | K(q) | q' \rangle, \] (3.7)

where \( \epsilon \) is an auxiliary simulation time step.

A necessary condition for \( W(q) \) to be a stationary distribution of this process is the differential equation

\[ K(q)W(q) = 0. \] (3.8)

On the other hand, Detailed Balance may be written as the operatorial equation

\[ K(q)W(q) = W(q)K^\dagger(q). \] (3.9)

Of course we cannot evaluate exactly the matrix elements of \( K \). This would be equivalent to solving exactly the quantum mechanical problem associated to the path-integral quantum extension of \( S(q) \).
Many algorithms arise in trying to approximate the kernel $K$. We consider now some well known proposals. The basic idea is to factorize approximately the kernel $K$ and to read the factorization as a succession of elementary steps in the update of the old Markov state.

**A. Langevin algorithm**

The standard Langevin algorithm splits $H = H_1 + H_2$ with

$$ H_1 = \frac{1}{\beta} \Pi^2, $$

$$ H_2 = i\Pi F(q). $$

Then

$$ P(q' \rightarrow q'') = \int d\xi \langle q''|e^{-\epsilon H_1}\xi\rangle\langle\xi|e^{-\epsilon H_2}|q'\rangle + O(\epsilon^2) $$

(3.11)

The sum over $\xi$ can be read as the composition of two successive updates realized with each of the two operators $H_1$ and $H_2$. They have trivial matrix elements in the coordinate representation [6].

$$ \langle q''|e^{-\epsilon H_1}|q'\rangle = \left(\frac{\beta}{2\pi\epsilon}\right)^{n/2} \exp\left[-\frac{\beta}{2\epsilon}(q'' - q')^2\right], $$

(3.12)

$$ \langle q''|e^{-\epsilon H_2}|q'\rangle = \delta(q'' - q(\epsilon)) $$

(3.13)

where $q(t)$ is defined by

$$ q(0) = q', \quad \dot{q}(t) = F(q). $$

(3.14)

The resulting explicit update is

$$ q'' = q(\epsilon) + \sqrt{\frac{2\epsilon}{\beta}} \xi, $$

(3.15)

where $\xi$ is a Gaussian random number with zero mean and unit variance.

This procedure introduces a systematic error in the construction of the statistical sample since the static distribution is now the zero mode of the operator $\bar{H}$ defined by
\[
\exp \left( -\epsilon H_1 \right) \exp \left( -\epsilon H_2 \right) = \exp \left( -\epsilon \bar{H} \right)
\]
\[\bar{H} = H + \epsilon \delta_1 H + \ldots. \tag{3.16}\]

Solving perturbatively in \( \epsilon \) the equation
\[ (H + \epsilon \delta_1 H + \ldots) (W + \epsilon \delta_1 W + \ldots) = 0 \tag{3.17} \]
we find a non trivial \( \delta_1 W \) which affects to order \( O(\epsilon) \) all the averages on the sample
\[ W + \epsilon \delta_1 W = \exp \left\{ -\beta \left[ S + \frac{\epsilon}{4} \left( \nabla^2 S - \beta (\nabla S)^2 \right) \right] \right\}. \tag{3.18} \]

Therefore, Detailed Balance holds exactly only with respect to \( \bar{H} \). Of course, we are not able to build explicitly the function \( q(t) \). At this order we can use
\[ q'' = q' + \epsilon F(q') + \sqrt{\frac{2\epsilon}{\beta}} \xi \tag{3.19} \]
and the only consequence is a different explicit form of the correction term which becomes now
\[ W + \epsilon \delta_1 W' = \exp \left\{ -\beta \left[ S + \frac{\epsilon}{4} \left( \nabla^2 S - \beta \left( \nabla S \right)^2 \right) \right] \right\}. \tag{3.20} \]

1. Smart Monte Carlo

In this section we show how the structure of the Detailed Balance violations in the Langevin algorithm (which the Smart Monte Carlo method \([7]\) tries to correct) suggests the extension of the dynamics in an enlarged \((q,p)\) space. In this wider space the diffusive process modifies some approximation of a canonical Hamiltonian evolution. The Langevin update is \((\epsilon \rightarrow \epsilon^2/2)\)
\[ q' = q + \frac{\epsilon^2}{2} F(q) + \epsilon \xi \tag{3.21} \]
corresponding to the transition probability in Eq. (3.12). The interesting point is that the parameter controlling Detailed balance violations
\[ x = \frac{W(q') \langle q'' | K(q) | q' \rangle}{W(q'') \langle q' | K(q) | q'' \rangle} \tag{3.22} \]
may be written

\[ x = \exp \left( H(q'', p'') - H(q', p') \right), \]  

(3.23)

where \( H(q, p) = S(q) + \frac{1}{2}p^2 \) and

\[ \begin{align*}
\dot{p} &= \xi, \\
q'' &= q' + \frac{\epsilon^2}{2} F(q') + \epsilon p', \\
p'' &= p' + \frac{\epsilon}{2} \left( F(q') + F(q'') \right),
\end{align*} \]  

(3.24)

and this set of equations can be recast in the form of a standard leap-frog symplectic integrator (see Appendix A)

\[ \begin{align*}
\dot{p} &= \xi, \\
\bar{p} &= p' + \frac{\epsilon}{2} F(q'), \\
q'' &= q' + \epsilon \bar{p}, \\
p'' &= \bar{p} + \frac{\epsilon}{2} F(q''),
\end{align*} \]  

(3.25)

The conclusion is that the equality \( x = 1 \) can be enforced improving the approximation of the evolution determined by \( H \).

\section*{B. Hyperbolic algorithm}

This is a clever proposal \cite{8} which improves the naive Langevin algorithm using the dynamics of the Kramers equation \cite{3,4}. We double the degrees of freedom \( q \to (q, p) \) and introduce the operator

\[ H = \frac{\gamma}{\beta} \Pi_p^2 + i\Pi_p(-\gamma p) + i\Pi_p F(q) + i\Pi_q p, \]  

(3.26)

where \( \gamma \) is an arbitrary parameter.

The proof of convergence to equilibrium given for the Fokker-Planck evolution cannot be applied. However, following \cite{8}, \( H \) determines a Hamiltonian flow in \((q, p)\) space with a
diffusion term in the \( p \) variables. Hence if a solution of \( \dot{u} = Hu \) is positive at \( t = 0 \), it remains positive at any time later as can also be seen from the representation of the time evolution of \( H \) in terms of a path-integral with positive measure. On the other hand, integrating by parts any eigenvector \( u_n \) with non zero eigenvalue we get

\[
\int dq \, dp \, u_n = 0 \tag{3.27}
\]

and assuming some eigenvalue with positive real part we contradict positivity of the evolution determined by \( H \).

We introduce an \( O(\epsilon) \) error by splitting \( H = H_1 + H_2 \) with

\[
H_1 = \frac{\gamma}{\beta} \Pi_p^2 + i\Pi_p(-\gamma p) + i\Pi_p F(q),
\tag{3.28}
\]

\[
H_2 = i\Pi_q p
\]

we can write down an approximated update for \( H \) obtained from \( H_1 \) and \( H_2 \)

\[
p'' = (1 - \epsilon\gamma)p' + \epsilon F(q') + \sqrt{\frac{2\epsilon\gamma}{\beta}} \xi',
\tag{3.29}
\]

\[
q'' = q' + \epsilon p'.
\tag{3.30}
\]

The equilibrium distribution is

\[
W(q, p) = \exp \left\{-\beta \left( \frac{1}{2} p^2 + S(q) + \epsilon S_1(q, p, \gamma) + \cdots \right) \right\}.
\tag{3.31}
\]

The parameter \( \gamma \) can be tuned to minimize the autocorrelation time of the observable which we are going to measure. Unlike the Langevin case, it is impossible to give an expression of \( S_1(q, p, \gamma) \) in the form of a polynomial in \( S(q) \) and its derivatives.

On the basis of the above general arguments we should have introduced a systematic error of order \( O(\epsilon) \) due to \( S_1(q, p, \gamma) \). This holds true for averages of generic functions \( \Omega(q, p) \) which depend on the auxiliary variables. However, if we are interested in functions \( \Omega(q) \) of \( q \) only, it is shown in [8] that the particular form of \( S_1(q, p, \gamma) \) reduces the error to \( O(\epsilon^2) \).

Assuming the \( q \) even under time reversal, the \( p \) variables must be are odd under \( T \). This implies that the Detailed Balance condition must be written [11]
\[ K(q,p)W(q,p) = W(q,p)K^\dagger(q, -p) \quad (3.32) \]

and in our case it is violated by \( O(\epsilon) \) terms because of \( S_1(q, p, \gamma) \).

An interesting variant of this procedure is called Guided Hybrid Monte Carlo [9], this is an algorithm which admits an exact extension and we shall discuss it later as a particular case of our methods.

IV. IMPROVED ALGORITHM

In this section we shall describe our approach which allows us for an improvement of the precision up to any desired order and which is a natural generalization of the previous schemes.

The key point of our method is a different operator splitting of \( H \). Indeed, we can separate \( H = H_{irr} + H_{rev} \) where

\[
H_{irr} = \frac{\gamma}{\beta} \Pi_p^2 + i\Pi_p(-\gamma p), \quad (4.1)
\]

\[
H_{rev} = i\Pi_p F(q) + i\Pi_q p. \quad (4.2)
\]

The important point is that both \( H_{irr} \) and \( H_{rev} \) annihilate the static distribution

\[
W(q, p) = \exp \left\{ -\beta \left( \frac{1}{2} p^2 + S(q) \right) \right\}. \quad (4.3)
\]

After all, this is why the Kramers equation works in the continuum limit. Writing

\[
\exp(-\epsilon H_{irr}) \exp(-\epsilon H_{rev}) = \exp(-\epsilon (H_{irr} + H_{rev} + \epsilon X)), \quad (4.4)
\]

the operator \( X \) is non trivial but has the useful property \( XW(q, p) = 0 \). This observation has the important consequence that we can consistently set to zero all the corrections in powers of \( \epsilon \) to \( W(q, p) \) and treat independently the irreversible and the reversible evolutions.

We expect Detailed Balance to hold exactly: indeed, as we have remarked above, the two kernels

\[
\exp(-\epsilon H_{irr}) \quad \exp(-\epsilon H_{rev}) \quad (4.5)
\]
leave invariant $W$ which is therefore a steady state for the evolution determined by any string $K$ of the form

$$K = \prod_i \exp(-a_i \epsilon H_{irr}) \exp(-b_i \epsilon H_{rev}), \quad (4.6)$$

where $a_i$ and $b_i$ are constants.

Indeed, we can check that separately

$$H_{irr}(q, p)W(q, p) = W(q, -p)H_{irr}^\dagger(q, -p), \quad (4.7)$$

$$H_{rev}(q, p)W(q, p) = W(q, -p)H_{rev}^\dagger(q, -p), \quad (4.8)$$

we conclude that the Detailed Balance condition is exactly satisfied by a symmetric splitting like for instance

$$K = \exp\left(-\frac{1}{2} \epsilon H_{irr}\right) \exp(-\epsilon H_{rev}) \exp\left(-\frac{1}{2} \epsilon H_{irr}\right). \quad (4.10)$$

Of course, we must specify how to evaluate the matrix elements of the two kernels, but this is not a problem. The irreversible part can be solved exactly. Writing

$$\Omega_1 = \frac{\gamma}{\beta} \Pi_p^2,$$  
$$\Omega_2 = i\Pi_p(-\gamma p), \quad (4.11)$$

then we obtain

$$[\Omega_1, \Omega_2] = -2\gamma \Omega_1 \quad (4.13)$$

and by the Campbell-Baker-Hausdoff formula

$$\exp(-\epsilon(\Omega_1 + \Omega_2)) = \exp(-h(\epsilon)\Omega_1) \exp(-\epsilon \Omega_2). \quad (4.14)$$

Differentiating with respect to $\epsilon$ with the condition $h(0) = 0$ we get

$$h(\epsilon) = \frac{1}{2\gamma} \left(1 - e^{-2\gamma \epsilon}\right). \quad (4.15)$$
The matrix element \( \langle p'', q' | p', q' \rangle_{irr} \) corresponds exactly to the discrete update

\[
p'' = e^{-\gamma \epsilon} p' + \sqrt{\frac{1 - e^{-2\gamma \epsilon}}{\beta}} \xi'. \tag{4.16}
\]

The reversible matrix element \( \langle p'', q'' | p', q' \rangle_{rev} \) must be some approximate integration of the deterministic Cauchy problem

\[
\dot{q} = p \quad \dot{p} = F(q) \tag{4.17}
\]

corresponding to the update

\[
q'' = Q(q', p', \epsilon) \quad p'' = P(q', p', \epsilon), \tag{4.18}
\]

where the maps \( Q \) and \( P \) can be, for instance, an higher order symplectic integrator. We stress that at this level of the discussion we do not need using a canonical integrator conserving the Poincaré invariants, in particular the phase-space measure. The importance of symplectic integrators will be clear in the discussion on the exact extensions of these algorithms.

We remark that the systematic error we are introducing is just the error made in approximating this reversible step. Its improvement is a well known problem which can be solved up to an arbitrary precision with increasing computational cost.

As in the hyperbolic algorithm, the free parameter \( \gamma \) can be tuned minimizing autocorrelations times, while the integration step \( \epsilon \) must be kept small enough to control systematic errors.

### A. Extended schemes

Following the above ideas, we can introduce schemes in which other free parameters are present. They can be tuned to obtain even smaller autocorrelations times. The simplest example is

\[
H = H_{irr} + H_{rev} + H_{rot}, \quad \tag{4.19}
\]
where

\[ H_{\text{irr}} = \frac{\gamma}{\beta} \Pi_y^2 + i\Pi_y(-\gamma y), \] (4.20)

\[ H_{\text{rev}} = i\Pi_p F(q) + i\Pi_q p, \] (4.21)

\[ H_{\text{rot}} = i\alpha (y\Pi_p - p\Pi_y). \] (4.22)

The operator \( H_{\text{rot}} \) is just a rotation in the \((y, p)\) plane and its exact matrix elements

\[ \langle p'' y'' \mid \exp(-\epsilon H_{\text{rot}}) \mid p' y' \rangle \] (4.23)

corresponds therefore to the update

\[ p'' = p' \cos(\alpha \epsilon) + y' \sin(\alpha \epsilon), \] (4.24)

\[ y'' = y' \cos(\alpha \epsilon) - p' \sin(\alpha \epsilon). \]

A symmetric kernel like

\[ \exp(-\epsilon H_{\text{irr}}) \exp(-\epsilon H_{\text{rot}}) \exp(-\epsilon H_{\text{rev}}) \exp(-\epsilon H_{\text{rot}}) \exp(-\epsilon H_{\text{irr}}) \] (4.25)

satisfies exactly the Detailed Balance condition with respect to the equilibrium distribution

\[ W(q, p, y) = e^{-\beta \left[ \frac{1}{2}(p^2 + y^2) + S(q) \right]}. \] (4.26)

The parameters \( \gamma \) and \( \alpha \) must be tuned, but we are unable to provide a general rule for their choice. However we shall show that the additional \( y \) variables improve the optimal autocorrelation of the algorithm.

An interesting feature of this scheme is that if we let \( y \) reach equilibrium, inserting one \( \exp(-\epsilon H_{\text{irr}}) \) factor near \( \exp(-\epsilon H_{\text{rev}}) \) and setting \( \gamma \to \infty \), then we obtain

\[ y' = \frac{1}{\sqrt{\beta}} \xi, \] (4.27)

\[ p' = p \cos(\alpha \epsilon) + \frac{1}{\sqrt{\beta}} \xi \sin(\alpha \epsilon) \]

which is just the mixing which we find in the stochastic step of the Guided Hybrid algorithm. It is clear that, at least formally, we reduce to this update starting from our basic \((q, p)\) scheme and relating \( \gamma \) to \( \alpha \) writing
\[
\exp(-\gamma \epsilon) = \cos(\alpha \epsilon) \quad 0 < \alpha \epsilon < \frac{\pi}{2} \quad (4.28)
\]

(the case in which the cosine is negative is handled easily by a slight generalization introduced in the following section).

A very natural extension is obtained building in the space \((q, p, y_1, \cdots, y_N)\) a chain of rotation operators acting in the space of the auxiliary variables

\[
H_{\text{rev}} = i \Pi_p F(q) + i \Pi_q p, \quad (4.29)
\]
\[
H_{\text{rot},1} = i \theta_1 (y_1 \Pi_p - p \Pi_{y_1}), \quad (4.30)
\]
\[
\cdots \quad (4.31)
\]
\[
H_{\text{rot},N} = i \theta_N \left( y_N \Pi_{y_{N-1}} - y_{N-1} \Pi_{y_N} \right), \quad (4.32)
\]
\[
H_{\text{irr}} = \frac{\gamma}{\beta} \Pi_{y_N}^2 + i \Pi_{y_N}(-\gamma y_N), \quad (4.33)
\]

where the angles \(\theta_i\) are free.

**B. Some remarks**

1. **Arbitrary rotations**

The reason why it is so natural to introduce the rotation operators \(H_{\text{rot}}\) is the following: if \(p\) be a \(N\)-component vector, then the discrete update

\[
p' = x C p' + \sqrt{1 - x^2} \xi \quad C \in \text{O}(N, \mathbb{R}) \quad (4.34)
\]

generates a normally distributed succession \(\{p\}\): \(P(p) = \exp \frac{1}{2} p^2\).

The connected component of this update may be written in terms of the exponential of \(\epsilon\) times a differential operator by introducing all the generators of \(\text{so}(N, \mathbb{R})\)

\[
H_{\text{rot}} = i \Theta_{ij} p_i \Pi_{p_j} \quad \Theta_{ij} = -\Theta_{ji}. \quad (4.35)
\]

The extended scheme of the previous section is just a particular choice of \(C\) realized as a chain of elementary rotations.
In the steps where the matrix element of the transition kernel are computed exactly, the parameter $\epsilon$ does not control an approximation any more. Indeed, our convergence analysis deals with the limit $\epsilon \to 0$ irrespectively of $\gamma \epsilon$, $\Theta_{ij} \epsilon$. On a formal level, one can take parameters $\gamma$ or $\Theta_{ij}$ not $O(1)$ with respect to $\epsilon$. From a practical point of view this means that we can choose $C$ independent of $\epsilon$; intuitively when the dynamics is switched off one is left with a free rotation in the $p$ space.

The vector $p$ may be the full set of generalized momenta in a single site. However, it can also mix momenta from different sites. This introduces long distance reshufflings and allows for pair-exchanges which are represented by orthogonal matrices.

2. Random parameters

In the Hybrid Monte Carlo [11,12], better autocorrelations may be obtained by randomizing the trajectory length. Here, a probability distribution for parameters like $\gamma$ may be

2 An interesting example of this mechanism if the following. We could try looking for an extension of the basic update

$$p'' = \alpha p' + \beta \xi \quad (4.36)$$

to the case $\alpha \in \mathbb{C}$ and $\beta$ to be determined. However, by complexifying $p$ and $\xi$ representing them as 2-vectors

$$p = u + iv \quad \xi = \eta + i p'' i \quad (4.37)$$

we have

$$p'' = |\alpha| C p' + \beta \xi \quad C = \frac{1}{|\alpha|} (\text{Re} \alpha - i \sigma_2 \text{Im} \alpha) \in O(2, \mathbb{R}) \quad \sigma_2 \text{ is a Pauli matrix} \quad (4.38)$$

and choosing $\beta = \sqrt{1 - |\alpha|^2}$ we fall in the above case, since $C$ may have a limit different from 1 as $|\alpha| \to 1$. 

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introduced. However, from preliminary numerical investigations we have indications that this device should not be a major improvement.

3. Dynamical Fermions

Consider a model with dynamical fermions. As is well known, in such a situation, the most expensive part of a lattice simulation is the inversion of the fermionic propagator. The time spent during this step becomes the natural unit of time. A fundamental parameter is then the number of inversions per sweep which we shall call \( R \). A common implementation of dynamical fermions \[11\] replaces the fermionic degrees of freedom with bosonic fields \( \chi \) which are updated by a heat-bath step. The refreshment frequency is relevant here. As an example, let us integrate the equations of motion by the simplest leap-frog scheme of Eq. (A18). If we refresh the \( \chi \) fields every \( k \) sweeps and if \( N_{md} \) is the number of molecular dynamics steps in each sweep, then

\[
R = N_{md} + \frac{1}{k}.
\]

In the Hybrid Monte Carlo one usually takes \( N_{md} \gg 1 \) and \( k = 1 \). In the schemes we have discussed one has always \( N_{md} = 1 \) so that taking \( k = 1 \) is twice slower than a large \( k \).

V. DISCUSSION OF CORRELATIONS

Consider a function \( \Omega(q) \) of the dynamical variables. The evolution in time of the sample average of \( \Omega \) is given by

\[
\frac{\partial}{\partial t} \Omega = -H^\dagger \Omega.
\]

Consider the continuum limit in which \( \epsilon \rightarrow 0 \) and let us compare the evolution of \( \langle q \rangle \) in the free theory where

\[
S(q) = \frac{1}{2} \omega^2 q^2
\]
for the three cases discussed above. We restrict the discussion to the case in which all the tunable parameters are independent of $\epsilon$ (see the discussion in paragraph (IV B 1)). We have explicitly

$$-H^\dagger_{lang} = \frac{1}{\beta} \partial_q^2 - \omega^2 q \partial_q,$$

$$-H^\dagger_{hyp} = \frac{1}{\beta} \partial_p^2 - \gamma p \partial_p - \omega^2 q \partial_p + p \partial_q,$$

$$-H^\dagger_{(q,p,y)} = \frac{1}{\beta} \partial_{y_N}^2 - \gamma y_N \partial_{y_N} + \sum_{i=1}^{N} \theta_i \left( y_i \partial_{y_{i-1}} - y_{i-1} \partial_{y_i} \right) - \omega^2 q \partial_p + p \partial_q,$$

$$y_0 = p).$$

The eigenvalues of the time evolution of $\langle q \rangle$ give directly the intrinsic autocorrelation of the Markov chain in the $\epsilon \to 0$ limit.

For the Langevin algorithm, we have a decay with eigenvalue $\lambda = -\omega^2$ and no possibility of tuning any parameter.

In the hyperbolic case, we have two eigenvalues $\lambda_+ \text{ and } \lambda_-$ and

$$\min_{\gamma} \max (\lambda_+, \lambda_-) = -\omega$$

obtained at $\gamma = 2\omega$. Dimensions are different with respect to Langevin, because the Kramers equation is second order; afterall, this is why the hyperbolic algorithm is better than the Langevin one.

In the $(q, p, y)$ extended scheme the roots of the secular equation $\lambda_i$ are tedious functions of $\theta_i$ and $\gamma$. We remark that a possible choice is to choose $\gamma$ and $\theta_i$ in such a way to have the maximum possible degeneracy in $\lambda$. Some explicit results for low values of $N$ are shown in Tab. I where all the variables has been made adimensional dividing out by $\omega$. One can improve the autocorrelation of $\langle q \rangle$ of at least a factor $\sqrt{11}$ in the $N = 5$ case. It seems reasonable that this mechanism can be improved with no limit introducing more and more auxiliary variables (up to $N < 6$ Tab. I) satisfies $\lambda_N = -\sqrt{2N+1}$ and we must balance the increasing computational work needed to tune all the associated new parameters and the gain in autocorrelation of the sample.
If we take into account the details of the discrete dynamics at $\epsilon > 0$ we obtain linear recursive equations giving the evolution of the momenta instead of differential equations. Their characteristic polynomials determine the $\epsilon$ dependent relaxation eigenvalues. For $\epsilon$ small enough the qualitative picture which one finds in the continuum does not change.

Of course, we cannot be too optimistic. In a realistic model there will be many relevant frequencies. An optimal tuning for all of them will average on their separate behaviours. Since we cannot give analytical estimates for autocorrelations in interacting models, explicit numerical tests are needed.

**A. Curved Space**

We are mainly interested in the generalization from flat space to the case of the curved manifold of a Lie group $G$. We must endow the configuration space with a definite metric and write down the corresponding covariant Fokker-Planck or Kramers equation. The most convenient and natural choice is the left and right invariant metric $ds^2 = \text{Tr}(dU \, dU^\dagger)$. Its Laplace-Beltrami invariant operator is built by substituting derivatives $\partial_\alpha$ with left-derivatives on the group $\nabla_\alpha$ defined by

$$f(\exp(ie^\alpha T^\alpha)g) = f(g) + \epsilon^\alpha \nabla_\alpha f(g) + O(\epsilon^2).$$

(5.5)

This choice is convenient because $\partial_\alpha$ was the generator of translations in flat space whereas on the group $\nabla_\alpha$ is simply the generator of translations by left multiplication $^L$. In the Langevin case, the diffusive term is the heat kernel

$$\langle g'|e^{-\epsilon^2}\nabla^2|g''\rangle = \langle 1|e^{-\epsilon^2}(g')^{-1}g''\rangle,$$

(5.6)

namely the matrix elements of the Laplace-Beltrami operator on $G$. For $SU(N)$ a compact expression can be given $^{10}$ which however is gaussian in the Lie parameters only if $g'$ is

$^3$We recall that dealing with $\nabla_\alpha$ we can integrate by parts with respect to the Haar measure $d\mu(g)$.
near to $g''$ (the weak coupling limit of $QCD$). The advantage of the Kramers equation is that it is associated to a diffusion on $R^n \times G$ where $n = \dim G$, the $p$ variables being flat. The molecular dynamics on the group is more complicated than in the flat case, but no curved heat kernel is needed here because the Hamiltonian evolution on $G$ is modified by a diffusion in its flat Lie algebra.

**VI. EXACT EXTENSIONS**

Until now we have considered methods which are not exact and need an extrapolation to obtain the exact $\epsilon \to 0$ limit. Moreover, finite $\epsilon$ effects can be studied by the analysis of the effects of the correction terms in the equilibrium action and it is not always clear if critical behaviour is unchanged if this terms are present. Nevertheless, they have some advantages over exact methods; on a formal level, they can deal with complex actions and they do not suffer the decrease of efficiency with increasing volume of the Hybrid Monte Carlo algorithm due to the acceptance rate.

Anyhow, adding a global accept/reject test, we can write exact extensions which satisfy the Detailed Balance condition. Let us consider the minimal $(q, p)$ scheme of the improved Hyperbolic algorithm; let us introduce an irreversible transition probability $\Pi$, a reversible one $T$ and an accept/reject test associated with the acceptance probability $A$. We want to prove Detailed Balance in full generality so we point out which properties of these components we need.

The irreversible transition probability must satisfy

$$\Pi(p' \to p'') = \Pi(-p' \to -p''), \quad (6.1)$$

$$\int \Pi(p' \to p'') \, dp'' = 1, \quad (6.2)$$

$$W(q, p')\Pi(p' \to p'') = W(q, p'')\Pi(p'' \to p'), \quad (6.3)$$

where we have put $\beta = 1$ and $W(q, p) = \exp(-S(q, p))$ is the equilibrium state.

The properties of the reversible transition probability are
\[\int T(q', p' \rightarrow q'', p'') \, dq'' \, dp'' = 1, \quad (6.4)\]
\[T(q', p' \rightarrow q'', p'') = T(q'', -p'' \rightarrow q', -p'). \quad (6.5)\]

The requirement on \(A\) is the following: define
\[K(q', p' \rightarrow q'', p'') = A(q', p' \rightarrow q'', p'') T(q', p' \rightarrow q'', p''), \quad (6.6)\]
then we want
\[W(q', p') K(q', p' \rightarrow q'', p'') = W(q'', p'') K(q'', -p'' \rightarrow q', -p'). \quad (6.7)\]

An explicit choice of \(\Pi, T\) and \(A\) which satisfies all the above conditions is
\[\Pi(p' \rightarrow p'') = c \exp \left[ \frac{1}{2(1 - x^2)} (p'' - xp')^2 \right],\]
\[T(q', p' \rightarrow q'', p'') = \delta(q'' - Q(q', p')) \delta(p'' - P(q', p')), \quad (6.8)\]
\[A(q', p' \rightarrow q'', p'') = \min\{1, W(q'', p'')/W(q', p')\},\]
where \(x\) is any real number and \(Q, P\) are the maps associated to a symplectic integrator.

The integrator must be canonical to avoid any Jacobian in verifying Eq. (6.5).

**A. \((q, p)\) scheme**

Our extension of the \((q, p)\) scheme is the following
\[(q', p') \xrightarrow{\Pi} (q', p_1),\]
\[(q', p_1) \xrightarrow{T} (q_1, p_2),\]
accept : \((q'', p_3) = (q_1, p_2)\) with \(P = A(q', p_1 \rightarrow q_1, p_2), \quad (6.9)\)
reject : \((q'', p_3) = (-p_1, q')\) with \(P = 1 - A(q', p_1 \rightarrow q_1, p_2),\]
\[(q'', p_3) \xrightarrow{\Pi} (q'', p'').\]

The full transition probability of the above algorithm is
\[ P(q', p' \rightarrow q'', p'') = \]
\[ \int \Pi(p' \rightarrow p_1)K(q', p_1 \rightarrow q'', p_2)\Pi(p_2 \rightarrow p'')
\]
\[ dp_1 \ dp_2 + \int \Pi(p' \rightarrow p_1)\{1 - A(q', p_1 \rightarrow q_1, p_2)\}T(q', p_1 \rightarrow q_1, p_2) \times \]
\[ \times \Pi(-p_1 \rightarrow p'')\delta(q' - q'') \ dp_1 \ dp_2 \ dq_1. \tag{6.10} \]

Using the properties of \( \Pi, T \) and \( A \) we verify the normalization condition

\[ \int P(q', p' \rightarrow q'', p'') \ dq'' \ dp'' = 1. \tag{6.11} \]

In Appendix we show that

\[ W(q', p')P(q', p' \rightarrow q'', p'') = W(q'', p'')P(q'', -p'' \rightarrow q', -p'), \tag{6.12} \]

hence Detailed Balance is demonstrated.

**B. \((q, p, y)\) scheme**

We restrict ourselves for simplicity to the \( N = 1 \) case. If we assume \( q \) even under time reversal, it follows that also \( y \) is even whilst \( p \) is odd. We expect to find a Detailed Balance equation of the form

\[ W(q', p', y')P(q', p', y' \rightarrow q'', p'', y'') = W(q'', p'', y'')P(q'', -p'', y'' \rightarrow q', -p', y'). \tag{6.13} \]

We must remember that the matrix element of \( H_{rot} \) in the \((p, y)\) plane is exact and leaves invariant the sum of squares in the action. Hence we have

\[ W(q', p', y')T_{rot}(q', p', y' \rightarrow q'', p'', y'') = W(q', p'', y'')T_{rot}(q', p', y' \rightarrow q'', p'', y''). \tag{6.14} \]

The scheme we propose is

\[ (q', p', y') \xrightarrow{\Pi} (q', p', y_1), \]
\[ (q', p', y_1) \xrightarrow{T_{rot}} (q', p_1, y_2), \]
\[ (q', p_1, y_2) \xrightarrow{T} (q_1, p_2, y_2), \]
accept : \( ( q'' , p_3 ) = ( q_1 , p_2 ) \) with \( P = A( q' , p_1 \rightarrow q_1 , p_2 ) \), \[ (6.15) \]

reject : \( ( q'' , p_3 ) = ( -p_1 , q' ) \) with \( P = 1 - A( q' , p_1 \rightarrow q_1 , p_2 ) \),

\[
( q'' , p_3 , y_2 ) \xrightarrow{T_{sym}} ( q'' , p'' , y_3 ),
\]

\[
( q'' , p'' , y_3 ) \xrightarrow{\Pi} ( q'' , p'' , y' ).
\]

In Appendix C we show that even for this scheme, the Detailed Balance condition in Eq. (6.13) holds.

VII. COMPARISON WITH HYBRID MONTE CARLO

Let us first consider the \((q, p)\) scheme. This algorithm has been tested on compact \(QED\) in \[9\] where its performance has been compared with the global Hybrid Monte Carlo.

In the \(\gamma \rightarrow \infty\) limit, we recover exactly the Hybrid Monte Carlo algorithm with a single molecular dynamics step. The quantity \((\gamma \epsilon)^{-1}\) plays qualitatively the role of \(N_{md}\) and a finite \(\gamma\) tries to reproduce a \(N_{md} > 1\) dynamics by taking into account the old momenta of the microcanonical evolution.

We remark that, after integrating out the fermions, the non local nature of the action prevents one from taking advantages from local Hybrid Monte Carlo algorithms \[14\]. The expected scaling behaviour is discussed as follows. Assume our lattice model to satisfy \(L \gg \xi\), where \(L\) is the lattice size and \(\xi\) the correlation length, then the acceptance probability of the HMC behaves as \(P_{\text{acc}} \sim \text{erfc}(cN_{md} \epsilon^3 \sqrt{V})\). Optimal tuning is expected to give \(N_{md} \sim 1/\epsilon\) with a sweep-sweep correlation \(\tau \sim 1/\epsilon\). To keep the acceptance rate constant while varying the volume needs the scaling \(\epsilon \sim V^{-1/4}\). The Kramers algorithm has \(N_{md} = 1\) independently on the tuning parameters. We assume that the scaling relation is modified to \(\epsilon \sim V^{-1/6}\); this assumption amounts to neglect the effects of momenta negation on the acceptance probability. If the optimal autocorrelations stay \(\sim 1/\epsilon\) then under our assumption, the HMC is expected to behave badly on larger volumes. Moreover, from the point of view of numerical precision, the opportunity of having \(N_{md} = 1\) is welcome; indeed, in \(QCD\), as
the volume \((L^4)\) grows or the quark mass \((m)\) is decreased we must have \(N_{md} \sim L/m^{3/4}\)
and some protection seems necessary to protect irreversibility against the accumulation of numerical errors.

The same qualitative discussion applies to the extended schemes. In a realistic model
many frequencies are present and the \(\lambda\) values of Tab. I are too optimistic. However, we
expect an improvement of efficiency with an appropriate tuning of \(\theta_i\) and the same qualitative
scaling with volume.

VIII. CONCLUSIONS

In summary, we have analyzed the Kramers equation approach to lattice simulations. Our
operatorial approach is an unified framework in which the convergence analysis is straightforward. Generalized algorithms come out easily with an increasing number of free parameters. They eventually can be tuned in order to minimize autocorrelations. Explicit numerical tests are needed. All these algorithms are particularly safe from the point of view of numerical precision and they are indicated when a great deal of computational effort is needed. Subsequent papers will be devoted to a numerical confirmation of the convergence and scaling properties of these proposals. In particular, we are interested in models with dynamical fermions where the numerical precision problem may be important.

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APPENDIX A: SYMPLECTIC METHODS

In this appendix we address the problem of the numerical canonical integration of the Hamilton equations. Many studies of this topic can be found in literature. Because of
its importance these works appear in many different research fields. We quote [14–16] as examples of papers belonging to the lattice field theory literature. However, similar investigations could be find for instance in [17] in a different context. An useful review for the reader may be [18] where specific features of the problem are discussed including \((i)\) non separable Hamiltonians \((ii)\) situations in which the computation of the derivatives of \(S(q)\) is not expensive.

We want to review shortly the techniques needed to build efficiently higher order approximation schemes. Let us consider a separable Hamiltonian \(H = T(p) + V(q)\) with \(N\) degrees of freedom. The symplectic 2-form \(\omega^2 = dp \wedge dq\) and its exterior powers \((\omega^2)^k\) with \(k = 1 \cdots N\) define the Poincaré invariant integrals which give invariant quantities when integrated; Liouville theorem is obtained with \(k = N\). We want to define a numerical map of initial conditions \((q_0, p_0)\) such that \(\omega^2\) is exactly preserved and the flow of \(H\) is approximated in some sense\(^4\).

Let \((q(\epsilon), p(\epsilon))\) the exact evolution of \((q_0, p_0)\) under \(H\). A symplectic integrator of order \(n\) is defined to be a canonical transformation \(\Phi\)

\[
(\tilde{q}_0, \tilde{p}_0) \xrightarrow{\Phi} (q, p, \epsilon)
\]  

(A1)

such that

\[
(q(\epsilon), p(\epsilon)) \xrightarrow{\Phi^{-1}} (\tilde{q}_0, \tilde{p}_0) = (q_0, p_0) + O(\epsilon^n).
\]  

(A2)

\(^4\) We remark that canonical integrators are intrinsically more stable than the non canonical ones, but they do not solve completely the problem of numerical stability. One would be tempted to apply KAM theory to conclude that a conserved new hamiltonian exists in the numerical evolution of the integrator. However, KAM theory does not apply here; as we shall see we are dealing with a Hamiltonian with discontinuous changes in time. Indeed, in \(N \geq 2\) degrees of freedom a large numerical diffusion may be observed (Arnold’s diffusion) even with canonical integrators. One usually expects this effect to be small, but in general there is no hope to catch the long time dynamics of \(H\).
Finding symplectic integrators is easy because of the following observation. Consider a canonical transformation \((q, p) \to (\tilde{q}_0, \tilde{p}_0)\) such that \((\tilde{q}_0, \tilde{p}_0) \to (q_0, p_0)\) as \(\epsilon \to 0\) and that the new Hamiltonian is
\[
H(\tilde{q}_0, \tilde{p}_0) = \sum_{k=n}^{\infty} h_k(\tilde{q}_0, \tilde{p}_0)\epsilon^k
\] (A3)
then the Hamiltonian evolution of \((\tilde{q}_0, \tilde{p}_0) \to (q_0, p_0)\) is zero up to order \(O(\epsilon^{n+1})\) and Eq. (A2) holds. Consider now the chain of canonical transformations
\[
(q_l, p_l) \xrightarrow{K_l} (q_{l-1}, p_{l-1}) \xrightarrow{K_{l-1}} \cdots \xrightarrow{K_1} (q_0, p_0),
\] (A4)
where the generating functions are
\[
K_i(q_{i-1}, p_i, \epsilon) = -q_{i-1}p_i - [a_i T(p_i) + b_i V(q_{i-1})].
\] (A5)
The explicit transformations are
\[
q_i = -\partial_{p_i} K_i = q_{i-1} + \epsilon a_i \partial_{p_i} T(p_i),
\]
\[
p_{i-1} = -\partial_{q_{i-1}} K_i = p_i + \epsilon b_i \partial_{p_{i-1}} V(q_{i-1}),
\] (A6)
\[
H_{i-1}(q_{i-1}, p_{i-1}) = H_i + \partial_t K_i.
\]
Imposing the validity of Eq. (A3) we obtain the desired symplectic integrators. We remark that the number of steps \(l\) grows faster than the order \(n\) like in standard Runge-Kutta schemes and finding higher order schemes by brute force is not possible. For the actual construction of symplectic integrators a different approach, namely the operatorial one, is more practical. Introducing the notation
\[
z = (q, p) \quad DGF = \{F, G\} = \sum_i \left( \frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} \right),
\] (A7)
the Hamilton equations are
\[
\dot{z} = D_H z \quad \Rightarrow \quad z(\epsilon) = \Phi_{\text{exact}}(\epsilon) z(0),
\] (A8)
where
\[ \Phi_{\text{exact}}(\epsilon) = \exp[\epsilon(A + B)] \quad A = D_{T(p)} \quad B = D_{V(q)} \] (A9)

and we have expressed the Hamiltonian evolution in terms of the exponential map of the sum of two differential (non commutative) operators. The explicit expression of \( \Phi_{\text{exact}} \) is not known in general. Again, an integrator of order \( n \) is a canonical approximation \( \Phi_n(\epsilon) \) of \( \Phi_{\text{exact}} \) exact to order \( O(\epsilon^n) \). Recalling Eq. (A5) we choose \( \Phi \) in the factorized form

\[ \Phi(\epsilon) = \prod_{i=1}^{k} e^{\epsilon c_i A} e^{\epsilon d_i B}. \] (A10)

The associated map \( z(0) \to z(\epsilon) \) corresponds as before to the chain of infinitesimal canonical transformations

\[ q_i = q_{i-1} + \epsilon c_i \partial_{q_{i-1}} T(p_{i-1}), \] (A11)

\[ p_i = p_{i-1} - \epsilon d_i \partial_{q_{i-1}} V(q_{i-1}). \] (A12)

The unknown constants \( \{c_i\} \) and \( \{d_i\} \) may of course be determined by brute force. However, a key observation which simplifies computation is that for any two operators \( A \) and \( B \) we have

\[ \exp \epsilon A \exp \epsilon B \exp \epsilon A = \exp \left\{ \epsilon (2A + B) + \frac{\epsilon^3}{6} ([B, [B, A]] - [A, [A, B]]) + O(\epsilon^5) \right\}. \] (A13)

If \( \Phi \) satisfies the time reversibility equation

\[ \Phi(-\epsilon) = \Phi^{-1}(\epsilon), \] (A14)

then \( \Phi \) does not have even terms

\[ \Phi(\epsilon) = \exp \left\{ \sum_{k=1}^{\infty} \epsilon^k X_k \right\} \quad \text{with} \quad X_2 = X_4 = \cdots = 0. \] (A15)

Using this property we can prove that given a symplectic integrator of order \( 2n \) satisfying Eq. (A14), the integrator

\[ \Phi_{2n+2}(\epsilon) = \Phi_{2n}(z_1 \epsilon) \Phi_{2n}(z_0 \epsilon) \Phi_{2n}(z_1 \epsilon) \] (A16)

is symplectic, satisfies Eq. (A14) and is of order \( 2(n+1) \) if and only if
\[
\begin{align*}
    z_0 &= -\frac{2^{1/(2n+1)}}{2 - 2^{1/(2n+1)}} \\
    z_1 &= \frac{1}{2 - 2^{1/(2n+1)}}.
\end{align*}
\]

(A17)

Since \(\Phi_2\) exists and is obtained using

\[
    k = 2 \quad c_1 = c_2 = \frac{1}{2} \quad d_1 = 1
\]

in Eq. (A10), we can show inductively that a reversible symplectic integrator of arbitrarily high order \(2n\) exists which involves \(3^{n-1} \Phi_2\) factors, namely \(3^{n-1} + 1\) elementary steps.

We remark that when high order integrators are needed, more direct approaches can save time. As an example, in [17] we find the proposal

\[
\Phi^{(m)} = \Phi_2(\epsilon w_m) \cdots \Phi_2(\epsilon w_0) \cdots \Phi_2(\epsilon w_m).
\]

(A19)

By a straightforward computation one finds that \(m = 3\) and \(m = 7\) are enough for the 6th and 8th order integrator. The constants \(\{w_i\}\) are given as numerical solutions of a set of algebraic equations. The reduced number of steps required is 8 and 16 in this case, whereas the scheme of Eq. (A10) needed 10 and 28 steps respectively.

**APPENDIX B: Proof of Eq. (6.12)**

We write

\[
W(q', p') P(q', p' \rightarrow q'', p'') = X_1 + X_2 + X_3
\]

(B1)

with

\[
X_1 = W(q', p') \int \Pi(p' \rightarrow p_1) K(q', p_1 \rightarrow q'', p_2) \Pi(p_2 \rightarrow p'') \ dp_1 \ dp_2,
\]

(B2)

\[
X_2 = W(q', p') \delta(q' - q'') \Pi^{(2)}(p' \rightarrow -p''),
\]

(B3)

\[
X_3 = -W(q', p') \int \Pi(p' \rightarrow p_1) K(q', p_1 \rightarrow q_1, p_2) \times
\]

\[
\times \Pi(-p_1 \rightarrow p'') \delta(q' - q'') \ dp_1 \ dp_2 \ dq_1,
\]

(B4)
where

\[ \Pi^{(2)}(p_1 \to p_2) = \int \Pi(p_1 \to p)\Pi(p \to p_2) \, dp. \] (B5)

Rewriting \( X_1 \) as

\[ X_1 = W(q'', p'') \int \Pi(p'' \to p_2)K(q'', -p_2 \to q', -p_1)\Pi(p_1 \to p') \, dp_1 \, dp_2 \] (B6)

it is clear that

\[ X_1(q', p' \to q'', p'') = X_1(q'', -p'' \to q', -p'). \] (B7)

The same property holds for \( X_2 \) since \( \Pi^{(2)} \) satisfies Detailed Balance like \( \Pi \) does. Finally

\[ X_3(q', p' \to q'', p'') = \]

\[ -\int dq_1 \, dp_1 \, dq_2 \, dp_2 \, \delta(q_2 - q')\delta(q_2 - q'')\Pi(p_1 \to p')\Pi(p_1 \to -p'') \times \]

\[ \times K(q_1, -p_2 \to q_2, -p_1)W(q_1, p_2) \]

from which it is evident that

\[ X_3(q', p' \to q'', p'') = X_3(q'', -p'' \to q', -p'). \] (B9)

**APPENDIX C: Proof of Eq. (6.13)**

We now proof Eq. (6.13). We write as before

\[ W(q', p', y')P(q', p', y' \to q'', p'', y'') = Y_1 + Y_2 + Y_3 \] (C1)

then

\[ Y_1 = W(q', p', y') \int \Pi(y' \to y_1)T_{rot}(y_1, p' \to y_2, p_1)K(q', p_1 \to q'', p_2) \times \]

\[ \times T_{rot}(y_2, p_2 \to y_3, p'')\Pi(y_3 \to y'') \, dp_1 \, dp_2 \, dy_1 \, dy_2 \, dy_3 \] (C2)

and we see that
Regarding $Y_2$

\[ Y_2 = W(q', p', y') \delta(q' - q'') \int \Pi(y' \to y_1) T_{rot}(y_1, p' \to y_2, p_1) T(q', p_1 \to q_1, p_2) \times T_{rot}(y_2, -p_1 \to y_3, p'') \Pi(y_3 \to y'') \, dq_1 \, dp_1 \, dp_2 \, dy_1 \, dy_2 \, dy_3 \]  
\hspace{1cm} (C4)

but

\[ \int T_{rot}(y_1, p' \to y_2, p_1) T_{rot}(y_2, -p_1 \to y_3, p'') \, dy_2 \, dp_1 = \]
\[ = \langle y_3, -p'' | e^{\epsilon H_{rot}} | y_2, p_1 \rangle \langle y_2, p_1 | e^{-\epsilon H_{rot}} | y_1, p' \rangle \, dy_2 \, dp_1 = \]  
\hspace{1cm} (C5)
\[ = \langle y_3, -p'' | y_1, p' \rangle = \delta(y_3 - y_1) \delta(p' + p'') \]

whence

\[ Y_2 = W(q', p', y') \delta(q' - q'') \delta(p' + p'') \Pi^{(2)}(y' - y'') \]  
\hspace{1cm} (C6)

and again

\[ Y_2(q', p', y' \to q'', p'', y'') = Y_2(q'', -p'', y'' \to q', -p', y'). \]  
\hspace{1cm} (C7)

Finally,

\[ Y_3 = W(q', p', y') \delta(q' - q'') \int \Pi(y' \to y_1) T_{rot}(y_1, p' \to y_2, p_1) K(q', p_1 \to q_1, p_2) \times T_{rot}(y_2, -p_1 \to y_3, p'') \Pi(y_3 \to y'') \, dq_1 \, dp_1 \, dp_2 \, dy_1 \, dy_2 \, dy_3 = \]  
\hspace{1cm} (C8)
\[ = \delta(q' - q'') \int \Pi(y_1 \to y') \Pi(y_3 \to y'') T_{rot}(y_1, p' \to y_2, p_1) T_{rot}(y_2, -p_1 \to y_3, p'') \times K(q_1, -p_2 \to q', -p_1) W(q', p_1, y_2) \, dq_1 \, dp_1 \, dp_2 \, dy_1 \, dy_2 \, dy_3. \]

Since in the motion determined by $H_{rot}$ we can view $y$ as a coordinate it follows that

\[ T_{rot}(y', p' \to y'', p'') = T_{rot}(y'', -p'' \to y', -p') \]  
\hspace{1cm} (C9)

We can verify that changing $p'$ and $p''$ into $-p''$, $-p'$ and exchanging the names of $y_1$ and $y_3$ the expression for $Y_3$ does not change.
REFERENCES

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[1] M. Beccaria, G. Curci and A. Viceré, Phys. Rev. E (accepted for publication).

[2] A. Sokal, Monte Carlo Methods in Statistical mechanics: Foundations and New Algorithms, in *Cours de Troisième Cycle de la Physique en Suisse Romande*.

  N. Madras and A.D. Sokal, Jour. of Stat. Phys. **50**, 109 (1988).

[3] H. A. Kramers, Physica **7**, 284 (1940)

[4] H. Risken, *The Fokker-Planck Equation*, Eds. Springer-Verlag, (1984).

[5] I.T. Drummond, S. Duane and R. R. Horgan, Nucl. Phys. B**220**, 119 (1983).

[6] S. A. Chin, Nucl. Phys. (Proc. Suppl.) B**9**, 498 (1989).

[7] P. J. Rossky, J. D. Doll and H. L. Friedman, J. Chem. Phys. **69**, 4628 (1978).

[8] A. M. Horowitz, Phys. Lett. **156**B, 89 (1985).

  A. M. Horowitz, Nucl. Phys. B**280**, 510 (1987).

[9] A. M. Horowitz, Phys. Lett. **268**B, 247 (1991).

[10] P. Menotti and E. Onofri, Nucl. Phys. B**190**, 288 (1981).

[11] S. Duane, A. D. Kennedy, B.J. Pendleton and D. Rowan, Phys. Lett. **195**B, 216 (1987).

[12] M. Creutz, Phys. Rev. D**38**, 1228 (1988).

  R. Gupta, G. W. Kilcup and S. R. Sharpe, Phys. Rev. D**38**, 1278 (1988).

  S. Gupta, A. Irback, F. Karsch and B. Petersson, Phys. Lett. **242**B, 437 (1990).

[13] P. Marenzoni, L. Pugnetti and P. Rossi, Parma University preprint, June 1993.

[14] M. Campostrini and P. Rossi, Nucl. Phys. B**329**, 753 (1990).
[15] M. Creutz and A. Gocksch, Phys. Rev. Lett. 63, 9 (1989).

[16] J. C. Sexton, D. H. Weingarten, Nucl. Phys. (Proc. Suppl.) B26, 613 (1992).

[17] H. Yoshida, Phys. Lett. A150, 262 (1990).

[18] R. I. McLachlan and P. Atela, Nonlinearity 5, 541 (1992).
### TABLE I. Some admissible $\gamma$, $\theta_i$ for the $(q, p, y)$ scheme

| $N$ | $\lambda$ | $\gamma$ | $\theta_1$ | $\theta_2$ | $\theta_3$ | $\theta_4$ | $\theta_5$ |
|-----|-----------|-----------|-------------|-------------|-------------|-------------|-------------|
| 1   | $-\sqrt{3}$ | $3\sqrt{3}$ | $2\sqrt{2}$ | $-$         | $-$         | $-$         | $-$         |
| 2   | $-\sqrt{5}$ | $4\sqrt{5}$ | $2$         | $5$         | $-$         | $-$         | $-$         |
| 3   | $-\sqrt{7}$ | $5\sqrt{7}$ | $4/\sqrt{5}$ | $7/\sqrt{5}$ | $\sqrt{56}$ | $-$         | $-$         |
| 4   | $-3$       | $18$      | $2\sqrt{7}$ | $\sqrt{\frac{243}{35}}$ | $\sqrt{\frac{36}{7}}$ | $\sqrt{105}$ | $-$         |
| 5   | $-\sqrt{11}$ | $7\sqrt{11}$ | $\sqrt{\frac{2}{3}}$ | $\frac{11}{\sqrt{21}}$ | $\sqrt{\frac{36}{7}}$ | $\sqrt{33}$ | $4\sqrt{11}$ |