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Computation within the auxiliary field approach ☆

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Abstract

Recently, the classical auxiliary field methodology has been developed as a new simulation technique for performing calculations within the framework of classical statistical mechanics. Since the approach suffers from a sign problem, a judicious choice of the sampling algorithm, allowing a fast statistical convergence and an efficient generation of field configurations, is of fundamental importance for a successful simulation. In this paper we focus on the computational aspects of this simulation methodology. We introduce two different types of algorithms, the single-move auxiliary field Metropolis Monte Carlo algorithm and two new classes of force-based algorithms, which enable multiple-move propagation. In addition, to further optimize the sampling, we describe a preconditioning scheme, which permits to treat each field degree of freedom individually with regard to the evolution through the auxiliary field configuration space. Finally, we demonstrate the validity and assess the competitiveness of these algorithms on a representative practical example. We believe that they may also provide an interesting possibility for enhancing the computational efficiency of other auxiliary field methodologies.

Keywords: Computational methods; Numerical methods; Monte Carlo methods; Analysis of algorithms and problem complexity; Classical equilibrium statistical mechanics

1. Introduction

During the last few years the auxiliary field methodology has undergone a fast development causing a considerable extension of its scope of application in physical and chemical research. Its underlying strategy is to map the many-particle problem onto one of independent particles interacting with an auxiliary field by using the complex Hubbard–Stratonovich (HS) transformation. The technique has so far primarily been used as an alternative approach to deal with quantum systems of fermions or bosons.

The so-called auxiliary field quantum Monte Carlo (AFQMC) method for fermionic systems uses the HS transformation to replace the exact imaginary-time propagator by an ensemble average of propagators of

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independent particles subjected to a time-dependent fluctuating auxiliary field. In this way the calculation of the exact energy is reduced to multiple independent calculations, each of which costs essentially the same as one Hartree–Fock iteration. The approach possesses two significant advantages over other ab initio quantum Monte Carlo methodologies: (1) that the antisymmetry of the multi-electron wave function is automatically incorporated and (2) that it is directly applicable to excited states. The technique has extensively been used to deal with strongly correlated systems of electrons like the Hubbard model [1,2]. It has then further be applied to electronic structure calculations of atoms and small molecules. However, its usefulness has severely been limited by strong convergence difficulties due to a numerical sign problem prohibiting its application to larger cases [3,4]. To overcome this instability, Rom et al. [5,6] proposed the shifted contour auxiliary field quantum Monte Carlo (SC-AFQMC) method. In this strategy the contour of integration of the functional integral is shifted into the complex plane by employing Cauchy's integral theorem. The path is chosen in a manner, so that it goes through the imaginary stationary point of the integral corresponding to the mean field (MF) solution. In this way a considerable acceleration of the statistical convergence of the Monte Carlo integration could be achieved, which has extended the range of application of AFQMC significantly.

Recently, another method based on the auxiliary field technique has been developed, the classical auxiliary field Metropolis Monte Carlo (AFMC) method [8–10], conceived for performing classical statistical simulations within an isothermal ensemble. It relies on the concept of recasting the conventional particle representation of the classical partition function in a field-theoretical formulation using the HS transformation. The motivation for developing this method was twofold [10]: (1) circumventing the particle insertion problem of traditional grand canonical Monte Carlo (GCMC) methods [11]. The difficulty manifests itself in a vanishingly small particle creation or destruction probability in systems of high density, thereby invalidating the algorithm. In the auxiliary field approach, the problem does not occur, since no particle insertion algorithm is employed; (2) providing a simulation tool for multi-scale modeling [12], thus opening the perspective for treating theories of different length scales within a unified framework.

The basic technique, however, suffers from a sign problem of the type also encountered in the AFQMC method, causing a bad statistical convergence of the thermodynamic averages in the low temperature and/or large system size regime. To reduce the difficulty, the AFMC method also involves strategies based on the contour-distortion technique. They rely on the concept of performing an exact transformation of the partition function integral by shifting the integration path in a way that it crosses or at least comes close to as many critical points as possible giving an important contribution to the overall entity. A suitable choice for the shift is gained with a specific selection procedure, which provides a new representation of the partition function. For the purpose of improving the statistical behavior of the grand canonical method two of such procedures have been devised. The first one uses the MF solution and leads to the mean field representation (MFR) of the partition function. It employs a similar strategy as the one adopted in the SC-AFQMC method of Rom et al. The second procedure utilizes the method of Gaussian equivalent representation, a sophisticated technique which was originally developed by Efimov and Ganbold [13] for the analytical approximation of functional integrals, and leads to its Gaussian equivalent representation (GER) [14]. An important aspect of both procedures is that they both provide strictly exact representations of the partition function [5,10,14] and they do not require any approximation for improving the convergence properties in the simulation.

So far, essentially analytical transformation methods have been considered, to reduce the computational costs of the auxiliary field methodology. In this paper we tackle the problem in a numerical way by taking into account its computational aspects. Here we report on various sampling algorithms, which allow a fast statistical convergence and an efficient generation of field configurations. Especially, we focus on a new preconditioning technique which permits to adjust them on the specific requirements of the auxiliary field configuration space.

This paper is organized as follows. First, we review the basic auxiliary field theory and the integral transformation techniques, to make the methodology amenable for simulation. Then, we give a recipe for performing an optimal reweighting and discuss the close connection between the statistical behavior of the method and the choice of the reference system. In the following two sections we consider the technical aspects and discuss the advantages and drawbacks of the standard algorithms for sampling the auxiliary field configuration space. Afterwards, we introduce our new force-based algorithms relying on multiple-move propagation strategies. Then, to further optimize the calculation, we describe a preconditioning scheme, which permits to adapt these algorithms to the characteristic properties of the phase space sampled. Finally, we demonstrate their applicability and assess their efficiency on a representative model system. To conclude, we summarize the main results and end with a brief outlook.

2. Classical auxiliary field theory

To derive the basic field representation of the grand canonical partition function, let us start with the classical canonical partition function in particle representation

$$Q(N,V,T) = \frac{1}{h^{3N}N!}\int\int \mathrm{d}\vec{R}^N\,\mathrm{d}\vec{P}^N \exp[-\beta H(\vec{R}^N,\vec{P}^N)], \tag{1}$$

where

$$H(\vec{R}^N,\vec{P}^N) = \sum_{I=1}^{N}\frac{\overrightarrow{P_I}^2}{2m_I} + \Phi(\vec{R}^N) \tag{2}$$

represents the Hamilton function and $\vec{R}^N$ and $\vec{P}^N$ the set of particle positions $\{\vec{R}_1,\ldots,\vec{R}_N\}$ and particle momenta $\{\vec{P}_1,\ldots,\vec{P}_N\}$, respectively. Under the assumption that the particles in the system interact through a two-body potential $\Phi(\vec{R}_I-\vec{R}_J)$, finite at zero distance, we can recast the canonical partition function in its basic field representation. For this, we first rewrite the potential energy $\Phi(\vec{R}^N)$ in Fourier series representation, which is quadratic with respect to the density coefficients. This results in

$$\Phi(\vec{R}^N) = \frac{1}{2}\sum_{\vec{G}}\rho^*(\vec{G})\Phi(\vec{G})\rho(\vec{G}) - \frac{1}{2}N\Phi(0), \tag{3}$$

where the coefficients of the potential are positive or negative depending on whether they describe the repulsive or attractive part. In the subsequent step the terms with $\Phi(\vec{G})>0$ are then linearized by applying the complex HS transformation [6]

$$\exp\left\{-\frac{a}{2}x^2\right\} = \sqrt{\frac{1}{2\pi a}}\int_{-\infty}^{\infty}\exp\left[-\frac{y^2}{2a} - \mathrm{i}xy\right]\mathrm{d}y, \tag{4}$$

where the real constant $a>0$, while the terms with $\Phi(\vec{G})<0$ are subjected to the real HS transformation obtained by substituting x with $\mathrm{i}x'$. Since the repulsive part of the potential results in a complex integrand, we can reasonably assume that it essentially determines the convergence behavior of the auxiliary field method. Therefore, in the further development we only take this part into account, which should be considered as the most unfavorable case.

After some simple algebra we then get the field representation of the canonical partition function in a complex distribution formulation. Using subsequently the relation between the grand canonical and canonical partition function [15],

$$\Xi(\mu, V, T) = \sum_{N=0}^{\infty} \exp[\beta\mu N] Q(N, V, T), \tag{5}$$

where μ denotes the chemical potential, we finally obtain the complex distribution formulation of the grand canonical partition function

$$\Xi(\mu, V, T) = \int \mathscr{D}\sigma_{\Phi} \exp\left[-\beta V_{\text{eff}}^{\mu VT} \right], \tag{6}$$

with the effective potential

$$V_{\text{eff}}^{\mu VT} = \frac{1}{2\beta^2} \sum_{\vec{G}} \sigma^*(\vec{G}) \Phi^{-1}(\vec{G}) \sigma(\vec{G}) - \frac{\chi}{\beta V} \int \exp[-\mathrm{i}\sigma(\vec{r})] \, \mathrm{d}\vec{r}, \tag{7}$$

where $\sigma(\vec{r})$ represents the grand canonical auxiliary field and $\mathscr{D}\sigma_{\Phi} \propto \mathrm{d}\sigma(\vec{G}=0) \prod_{\vec{G}>0} \mathrm{d}\sigma^{\mathrm{R}}(\vec{G}) \mathrm{d}\sigma^{\mathrm{I}}(\vec{G})$ the field measure. The constant χ is a parameter depending on μ through the relation

$$\chi = \frac{V}{\lambda_{\mathrm{B}}^3} \exp\left[\beta\mu + \frac{1}{2}\beta\Phi(0) \right]. \tag{8}$$

This formulation of the grand canonical partition function, however, does not permit the crude application of the standard multi-dimensional integration techniques, like the Metropolis Monte Carlo (MC) algorithm. The problem is related to the complex nature of the Boltzmann-factor, which causes a bad statistical convergence of the thermodynamic quantities. Thus, to make the methodology amenable for computation, the contour-distortion technique based on Cauchy's integral theorem [16] has to be applied. It consists in distorting the integration path of the integral into the complex plane in such way that it passes through or at least comes close to its critical points. In practice, this is achieved by adding a constant shift to each field degree of freedom according to the prescription

$$\sigma^{\mathrm{R/I}}(\vec{G}) \to \sigma^{\mathrm{R/I}}(\vec{G}) + \mathrm{i}\psi^{\mathrm{R/I}}(\vec{G}). \tag{9}$$

This leads then to the contour-distorted grand canonical partition function in complex distribution formulation. For the purpose of the simulation the grand canonical partition function in complex distribution formulation has further to be recasted in a real distribution formulation. Using the fact that the partition function is a purely real quantity, we finally obtain the contour-distorted grand canonical partition function in real distribution formulation

$$\Xi(\mu, V, T) = \exp\left[\frac{1}{2\beta} \sum_{\vec{G}} \psi^*(\vec{G}) \Phi^{-1}(\vec{G}) \psi(\vec{G}) \right] \int \mathscr{D}\sigma_{\Phi} \cos\left(\beta V_{\text{eff}}^{\mathrm{I}/\mu VT} \right) \exp\left[-\beta V_{\text{eff}}^{\mathrm{R}/\mu VT} \right], \tag{10}$$

where

$$V_{\text{eff}}^{\mathrm{R}/\mu VT} = \frac{1}{2\beta^2} \sum_{\vec{G}} \sigma^*(\vec{G}) \Phi^{-1}(\vec{G}) \sigma(\vec{G}) - \frac{\chi}{\beta V} \int \exp[\psi(\vec{r})] \cos(\sigma(\vec{r})) \, \mathrm{d}\vec{r}, \tag{11}$$

$$V_{\text{eff}}^{\mathrm{I}/\mu VT} = \frac{1}{\beta^2} \sum_{\vec{G}} \psi^*(\vec{G}) \Phi^{-1}(\vec{G}) \sigma(\vec{G}) + \frac{\chi}{\beta V} \int \exp[\psi(\vec{r})] \sin(\sigma(\vec{r})) \, \mathrm{d}\vec{r}, \tag{12}$$

represent the real and imaginary part of the effective potential, respectively. With the objective of ameliorating the convergence behavior of the methodology, two procedures for judiciously selecting the shifting function have been developed, the MFR and GER procedure. In this work the more efficient GER

approach has been used for testing and assessing the efficiency of our algorithms. For a detailed discussion of these strategies and their convergence properties we refer to [8–10].

3. Computational aspects

3.1. Choosing the reference system

Within the classical auxiliary field approach the thermodynamic average of a physical property A can be expressed in the general form

$$\langle A\rangle = \frac{\int \mathscr{D}\sigma \mathscr{A}[\sigma]\rho[\sigma]}{\int \mathscr{D}\sigma \rho[\sigma]}, \tag{13}$$

where $\mathscr{D}\sigma$ represents the field integration measure and $\mathscr{A}[\sigma]$ the estimator belonging to the real and non-positive definite distribution $\rho[\sigma]$. It is a well-known fact that the computation of averages in the presence of such a distribution poses a practical problem. The standard numerical integration techniques, such as the MC algorithm, cannot be used directly for sampling, since they make sense only for real and positive distributions [17]. The common approach in such a case is to employ a reweighting procedure, which consists in factorizing the original distribution into a real and positive part, called the reference distribution, and a remainder, which is included in the estimator. The ensemble average of the property A is then calculated by evaluating the following expression:

$$\langle A\rangle = \left\{ \int \mathscr{D}\sigma \mathscr{A}[\sigma] \frac{\rho[\sigma]}{\rho^{\mathrm{ref}}[\sigma]} \rho^{\mathrm{ref}}[\sigma] \right\} \Big/ \left\{ \int \mathscr{D}\sigma \frac{\rho[\sigma]}{\rho^{\mathrm{ref}}[\sigma]} \rho^{\mathrm{ref}}[\sigma] \right\} = \left\langle \mathscr{A}[\sigma] \frac{\rho[\sigma]}{\rho^{\mathrm{ref}}[\sigma]} \right\rangle^{\mathrm{ref}} \Big/ \left\langle \frac{\rho[\sigma]}{\rho^{\mathrm{ref}}[\sigma]} \right\rangle^{\mathrm{ref}}, \tag{14}$$

where the brackets $\langle \cdots \rangle^{\mathrm{ref}}$ denote the average taken with respect to the real and positive definite reference distribution $\rho^{\mathrm{ref}}[\sigma]$. In practice, the averages in the numerator and denominator are approximated by their respective discrete sum [11]

$$\langle A\rangle \approx \lim_{\tau_{\mathrm{run}}\to\infty} \left\{ \sum_{i=1}^{\tau_{\mathrm{run}}} \mathscr{A}[\sigma_i] \frac{\rho[\sigma_i]}{\rho^{\mathrm{ref}}[\sigma_i]} \right\} \Big/ \left\{ \sum_{i=1}^{\tau_{\mathrm{run}}} \frac{\rho[\sigma_i]}{\rho^{\mathrm{ref}}[\sigma_i]} \right\}, \tag{15}$$

where τ_{run} defines the total number of auxiliary field configurations sampled from the reference distribution with a suitable sampling procedure. A crucial aspect for the evaluation of $\langle A\rangle$ is to find the reference distribution, which minimizes the standard deviations of the averages of the numerator and denominator and is independent of the estimator $\mathscr{A}[\sigma]$. A solution to the problem is obtained through the application of the variational method, which provides the absolute value of ρ [18],

$$\rho^{\mathrm{ref}}[\sigma] = \frac{|\rho[\sigma]|}{\int \mathscr{D}\sigma |\rho[\sigma]|} \tag{16}$$

and thus the average of the sign in the denominator of Eq. (14),

$$\langle \mathrm{sign}(\rho[\sigma])\rangle^{\mathrm{ref}} = \frac{\int \mathscr{D}\sigma \rho[\sigma]}{\int \mathscr{D}\sigma |\rho[\sigma]|}, \tag{17}$$

with the optimal SD

$$\sigma(\langle \mathrm{sign}(\rho[\sigma])\rangle^{\mathrm{ref}}) = \sqrt{1 - \langle \mathrm{sign}(\rho[\sigma])\rangle^{\mathrm{ref}^2}}. \tag{18}$$

The sampling technique, relying on this choice of the reference distribution, will in the following be referred to as the conventional procedure and the corresponding distribution as the conventional distribution. Note also that all the auxiliary field simulations of this work have been performed employing this procedure, unless explicitly specified otherwise. The sign problem now occurs when the average of the sign is vanishingly small and, unless a huge number of configurations is sampled, its large statistical fluctuations render the measurement meaningless. Finally, it is also worth stressing that the appropriate choice for the reference distribution depends mainly on the external conditions imposed on the system and therefore in some cases also other choices may be useful.

3.2. Sampling the auxiliary field configuration space

A successful simulation within the auxiliary field approach requires a judicious selection of the sampling algorithm, allowing a fast statistical convergence and an efficient generation of field configurations. There are essentially two points to take into account: (1) the correlation of the configurations, entering the variances of the numerator and denominator [19], and (2) the computational expense required, to generate them. It is clear that an ideal algorithm would be one which generates a sequence of configurations only slightly correlated at low computational cost.

In our subsequent investigation we will consider the following algorithmic alternatives:

1. Gaussian random numbers
2. Metropolis Monte Carlo
3. Molecular dynamics
4. Mixed molecular dynamics/Monte Carlo

To begin, let us first analyze the expression of the grand canonical partition function given in Eq. (10). An obvious simple possibility appears directly from the shape of the original distribution $\rho[\sigma]$ and consists in evaluating the ensemble average of the physical property A by generating configurations with respect to the Gaussian distribution

$$\rho^{\mathrm{ref}}[\sigma] \propto \exp\left[-\frac{1}{2\beta}\sum_{\vec{G}}\sigma^{*}(\vec{G})\Phi^{-1}(\vec{G})\sigma(\vec{G})\right]. \tag{19}$$

The technique is called the auxiliary field Gaussian random number (AFGRN) algorithm which is of similar type as the one commonly employed in AFQMC calculations [5,20]. At first sight it seems particularly attractive, because of the easy implementation and the fast generation of configurations. In addition, no data correlation must be considered in the averaging procedure, since all the configurations are statistically independent. We applied this technique to the computation of our auxiliary field functional averages and found that it works best in the high temperature and/or small system size regime, where the reference system is a good approximation to the system of interest. However, at lower temperatures and/or larger system sizes this reference system is inadequate, because the statistics are significantly deteriorated due to the occurrence of the sign problem. This renders the AFGRN algorithm very inefficient under these external conditions.

We already know from Section 3.1 that the best estimator-independent choice for the reference distribution is provided by the conventional procedure, i.e.,

$$\rho^{\mathrm{ref}}[\sigma] \propto \exp\left[-\beta V_{\mathrm{eff}}^{\mathrm{ref}}\right], \tag{20}$$

with the reference effective potential defined as

$$V_{\mathrm{eff}}^{\mathrm{ref}} = V_{\mathrm{eff}}^{\mathrm{R}} - \frac{1}{\beta}\ln\left|\cos(\beta V_{\mathrm{eff}}^{\mathrm{I}})\right|, \tag{21}$$

where $V_{\mathrm{eff}}^{\mathrm{R}}$ and $V_{\mathrm{eff}}^{\mathrm{I}}$ represent the real and imaginary part of the effective potential given through the Eqs. (11) and (12), respectively. By analyzing the above expression for $V_{\mathrm{eff}}^{\mathrm{ref}}$, we can easily deduce that its hypersurface

can be described by isolated valleys separated by infinite logarithmic barriers. Thus, the situation we have to deal with is a distribution with a discontinuous configuration space. For an efficient sampling of such a distribution, we must regard two important aspects: (1) our sampling technique has to circumvent the problem of ergodicity, i.e., it must be able to cross the barriers without difficulties, so that the system can reach the equilibrium; (2) it must permit to sample efficiently all the relevant parts of the phase space belonging to $\rho^{\mathrm{ref}}[\sigma]$.

An appropriate method for such purposes is the MC algorithm which was originally developed by Metropolis et al. [21]. It is a purely stochastic algorithm, which relies on the concept of importance sampling causing that the phase space trajectory migrates preferentially among the states, where the Boltzmann weight of the reference system is large. The technique constructs a Markov process [11,22], to generate a sequence of configurations with the desired distribution. It generally consists of two steps:

Step 1. Choose a new configuration σ_n with probability α_{mn} by randomly displacing a single degree of freedom at a time.

Step 2. Accept σ_n with probability $\pi_{A/mn}$ as a member of the Markov chain or reject it and keep the old configuration σ_m instead.

A suitable scheme for constructing such a sequence involves choosing a transition matrix π, which satisfies the condition of microscopic reversibility, $\rho_m\pi_{mn} = \rho_n\pi_{nm}$, and the normalization condition, $\sum_n \pi_{mn} = 1$, simultaneously. One such scheme has been suggested by Metropolis et al. [21] and is commonly known as the asymmetrical solution [11]. Now, employing this method in conjunction with the fast Fourier transformation (FFT) technique, to efficiently calculate the effective potential and the field estimators, provides us the so-called auxiliary field Metropolis Monte Carlo AFMC method. In order to be useful for auxiliary field computation, it is crucial that this method generates a trajectory, which hits several times the relevant states of the system of interest located around the critical points of the partition function integral. In practice, it appears that, as long as only a few degrees of freedom are required to accurately describe the physical system, this algorithm represents a viable procedure for accelerating the statistical convergence of the auxiliary field methodology.

A disadvantage of the original Metropolis algorithm, in cases when one has to deal with many field degrees of freedom, is that only one degree of freedom at a time is moved, to generate a new state. This may be changed so that several or all the degrees of freedom are moved simultaneously. Such a strategy has been adopted by Chapman and Quirke [23], who were able to demonstrate that with multiple-move propagation the equilibration of many-particle systems can be achieved more rapidly. However, a major problem of their approach is that the acceptance rate of the Metropolis procedure is drastically lowered with increasing number of degrees of freedom and we can reasonably expect that the same phenomenon would equally appear, if we would utilize it in conjunction with our auxiliary field methodology. In our case, the use of a force-based approach seems to be much more appropriate. Although such a strategy is certainly more expensive per cycle due to the force computation, it should nevertheless represent a major improvement, because the forces guide the sampling to the important regions of phase space and thus the field degrees of freedom are no longer randomly updated.

The basic concept of the force-based approach is to recast the average of a functional $\mathscr{O}$ in an expression, which is isomorphic to an average in the canonical ensemble. This is achieved by introducing for each field degree of freedom σ_i a momentum $p_{\sigma/i}$ and reformulating the average according to [24,25]

$$\langle \mathscr{O} \rangle = \langle \mathscr{O} \rangle_{\mathrm{canon}}, \tag{22}$$

where

$$\langle \mathscr{O} \rangle = \frac{\int \mathscr{D}\sigma \mathscr{O}[\sigma] \exp\left[-\beta V_{\mathrm{eff}}^{\mathrm{ref}}[\sigma]\right]}{\int \mathscr{D}\sigma \exp\left[-\beta V_{\mathrm{eff}}^{\mathrm{ref}}[\sigma]\right]} \tag{23}$$

is the average of $\mathcal{O}$, while

$$\langle \mathcal{O} \rangle_{\text{canon}} = \frac{\int \mathcal{D}p_\sigma \int \mathcal{D}\sigma \mathcal{O}[\sigma] \exp\left[-\beta H_{\text{eff}}^{\text{ref}}[p_\sigma, \sigma]\right]}{\int \mathcal{D}p_\sigma \int \mathcal{D}\sigma \exp\left[-\beta H_{\text{eff}}^{\text{ref}}[p_\sigma, \sigma]\right]} \tag{24}$$

defines the average of $\mathcal{O}$ with respect to the resulting canonical distribution. The function

$$H_{\text{eff}}^{\text{ref}}[p_\sigma, \sigma] = E_{\text{kin}}[p_\sigma] + V_{\text{eff}}^{\text{ref}}[\sigma] \tag{25}$$

represents the Hamiltonian consisting of the reference effective potential $V_{\text{eff}}^{\text{ref}}[\sigma]$ and the kinetic energy

$$E_{\text{kin}}[p_\sigma] = \sum_{i=1}^{N_\sigma} \frac{p_{\sigma/i}^2}{2m_{\sigma/i}}, \tag{26}$$

where N_σ is the total number of degrees of freedom and $m_{\sigma/i}$ the mass corresponding to the ith one.

To evaluate the above canonical ensemble average in a purely deterministic fashion, the extended system molecular dynamics (ESMD) method of Nosé [26] can be employed. The technique makes use of an additional degree of freedom s, which acts as an external heat bath on the physical system, to adjust the particle kinetic energy to the desired average value. During an ESMD simulation the augmented set of degrees of freedom is evolved dynamically through the extended phase space, thereby producing a trajectory over which the desired time averages are then estimated. To relate a time average of an observable $\mathcal{O}$ to its corresponding canonical ensemble average, the method employs the concept of the quasi-ergodic hypothesis [11]. The desired expectation value is finally recovered by taking into account relation (22). In a mathematical formulation this can be expressed in the following way:

$$\lim_{\tau_{\text{run}} \to \infty} \langle \mathcal{O} \rangle_{\tau_{\text{run}}}^{\text{ESMD}} = \langle \mathcal{O} \rangle_{\text{canon}}^{\text{ESMD}} = \langle \mathcal{O} \rangle_{\text{canon}} = \langle \mathcal{O} \rangle \tag{27}$$

with the time average defined as

$$\langle \mathcal{O} \rangle_{\tau_{\text{run}}}^{\text{ESMD}} = \frac{1}{(\tau_{\text{run}} - \tau_0)} \int_{\tau_0}^{\tau_{\text{run}}} \mathcal{O}[\sigma(s)]\, \mathrm{d}s, \tag{28}$$

where the estimator $\mathcal{O}$ is assumed to be a function of the set of auxiliary field degrees of freedom $\sigma(s)$ depending implicitly on the heat bath variable s. Such an approach was already employed by Kogut and Sinclair [27] for the simulation of lattice systems of quantum chromodynamics. An alternative to the purely deterministic approach is to combine the Newtonian dynamics with the stochastic collision thermostat of Andersen [28]. This strategy couples a heat bath to the physical system by introducing stochastic forces that act on the particles of the sample and change their kinetic energy. In practice, at intervals, the value of the momentum of a randomly selected particle is chosen afresh from the Maxwell–Boltzmann distribution with the desired average kinetic energy. This corresponds to a collision with an imaginary heat bath particle. An alternative to considering only one particle at a time is to select the momenta of all particles at once, i.e., to perform massive stochastic collisions. Such a technique has been employed by Andrea et al. [29]. An obvious advantage of these stochastic thermostating procedures over the deterministic one is that the randomization prevents the system trajectory to be trapped in the bottlenecks of phase space and therefore helps to satisfy the condition of ergodicity. This is a useful property, especially if one has to sample a hypersurface with a large amount of local minima, such as in case of the auxiliary field approach.

However, all these algorithms, if employed within the conventional procedure, would always suffer from their inability to overcome the logarithmic barriers. The hybrid Monte Carlo (HMC) method of Duane et al. [22] copes with the difficulty by making use of the integration errors introduced through finite difference approximation of the trajectory. The method combines the advantages of the molecular dynamics

(MD) method with those of the MC method. [1] In essence, the algorithm consists in numerically integrating Hamilton's equations of motion and thereby propagating the system trajectory a predefined number of time steps. Under the assumption that the time step is large enough, to get a reasonable energy drift, the final state of the sequence is accepted or rejected by performing a Metropolis test. If the new state is accepted as a member of the Markov chain, the trajectory continues to evolve through phase space untouched, otherwise new velocities are sampled from a Maxwell–Boltzmann distribution and the direction of the trajectory is changed. The Metropolis procedure removes the integration errors and thereby makes the algorithm exact. In practice, the time step is usually chosen as large as possible and is only restricted by the Metropolis acceptance rate, which should be kept satisfactory high. This enables a fast propagation through phase space and permits to pass through the logarithmic barriers. However, the usefulness of the algorithm depends on the size of the hurdle that has to be taken by the trajectory. Consequently, a good compromise between acceptance rate and ergodicity must be found which is not always possible. Furthermore, it can never be guaranteed that all the regions are really accessed, unless the phase space is everywhere of equal shape. This increases the need for the development of new algorithms, to overcome such difficulties.

In the following we propose two new classes of force-based algorithms for auxiliary field computation, which permit to cope with the problems mentioned previously, while preserving at the same time the advantages of multiple-move propagation.

3.3. Force-based auxiliary field algorithms

Their underlying concept relies on a reweighting strategy and consists in splitting the reference distribution $\rho^{\mathrm{ref}}[\sigma]$ of the ensemble average of a physical property A,

$$\langle A\rangle = \frac{\int \mathscr{D}\sigma \mathscr{A}[\sigma]\rho[\sigma]}{\int \mathscr{D}\sigma\rho[\sigma]} = \left\{ \int \mathscr{D}\sigma \mathscr{A}[\sigma] \frac{\rho[\sigma]}{\rho^{\mathrm{ref}}[\sigma]} \rho^{\mathrm{ref}}[\sigma] \right\} \Big/ \left\{ \int \mathscr{D}\sigma \frac{\rho[\sigma]}{\rho^{\mathrm{ref}}[\sigma]} \rho^{\mathrm{ref}}[\sigma] \right\}, \tag{29}$$

in a sampling distribution $\rho^{\mathrm{samp}}[\sigma]$ and a remaining distribution $\rho^{\mathrm{rest}}[\sigma]$,

$$\langle A\rangle = \left\{ \int \mathscr{D}\sigma \mathscr{A}[\sigma] \frac{\rho[\sigma]}{\rho^{\mathrm{ref}}[\sigma]} \rho^{\mathrm{rest}}[\sigma]\rho^{\mathrm{samp}}[\sigma] \right\} \Big/ \left\{ \int \mathscr{D}\sigma \frac{\rho[\sigma]}{\rho^{\mathrm{ref}}[\sigma]} \rho^{\mathrm{rest}}[\sigma]\rho^{\mathrm{samp}}[\sigma] \right\}. \tag{30}$$

The average is then calculated as follows:

Step 1. Start from a configuration σ_m, which belongs to the configuration space of $\rho^{\mathrm{ref}}[\sigma]$, and propagate the system from state σ_m to state σ_n by using an algorithm, which generates configurations from $\rho^{\mathrm{samp}}[\sigma]$.

Step 2. Check if σ_n also belongs to the configuration space of $\rho^{\mathrm{ref}}[\sigma]$ by performing an additional acceptance/rejection step with regard to $\rho^{\mathrm{rest}}[\sigma]$. This can be done either with a Metropolis or a von Neumann procedure.

As we can easily convince ourselves this strategy possesses all the advantageous features for cases where one has to deal with a distribution having a discontinuous configuration space, such as in the auxiliary field methodology. It permits, on one hand, to recover the conventional reference distribution and, on the other, to solve the ergodicity problem, which is a fundamental requirement to obtain reliable results from the simulation [11].

The first technique we propose in the following utilizes the HMC method [22], to generate field configurations from a suitably selected sampling distribution, and a supplementary Metropolis step, to test whether they also belong to the configuration space of the reference distribution. We call the new algorithm

[1] For a review of this or related methods we refer to [30].

the Metropolis auxiliary field hybrid Monte Carlo (MS-AFHMC) method. A variant of it neglects the correction step of the HMC method and is called the Metropolis auxiliary field hybrid molecular dynamics (MS-AFHMD) method. The second technique is based on the concept of the von Neumann rejection algorithm [11,31], which also relies on a two-step procedure. First, a configuration from a judiciously chosen sampling distribution is generated, which is then submitted to a von Neumann rejection step, to test whether it also belongs to the space of the reference distribution. Combined with the HMC or massive stochastic collision algorithm the new technique is called either the von Neumann auxiliary field hybrid Monte Carlo (VN-AFHMC) method or the von Neumann auxiliary field hybrid molecular dynamics (VN-AFHMD) method.

We finally demonstrate the validity and assess the competitiveness of these algorithms on a system of particles interacting through a purely repulsive Gaussian potential [32]. The choice of the so-called Gauss-core (G) potential, $\Phi_G(\vec{r}) = \Phi_G(0)\exp[-(\vec{r}/l)^2]$, has been particularly motivated by the assumption that the convergence difficulties are essentially caused by the repulsive part of the interaction due to the introduction of the complex HS transformation. Moreover, it gives a good description of the repulsive contribution of interactions encountered in realistic systems and fulfills all the necessary requirements to ensure the validity of the auxiliary field methodology. Note finally that all the results presented in the following are expressed in reduced Gauss-core units, a system of units that is natural for the model.

3.3.1. The Metropolis procedure

We now consider in more detail the first case where we generate a sequence of configurations from $\rho^{\text{ref}}[\sigma]$ by constructing a Markov process. Under the assumption of ergodicity, this process will converge in the long-time limit to the desired limiting distribution, while fulfilling the condition of microscopic reversibility

$$\rho_m^{\text{ref}}\pi_{mn}^{\text{ref}} = \rho_n^{\text{ref}}\pi_{nm}^{\text{ref}}, \tag{31}$$

as well as the normalization condition

$$\sum_n \pi_{mn}^{\text{ref}} = 1. \tag{32}$$

Here, π_{mn}^{ref} defines the transition probability to reach the state σ_n starting from σ_m, within the reference state space, using an as yet unspecified procedure, while ρ_m^{ref} represents the probability of the system to be in state σ_m. In order to construct the Markov process, we define π_{mn}^{ref} as follows:

$$\pi_{mn}^{\text{ref}} = \pi_{mn}^{\text{samp}}\pi_{mn}^{\text{rest}}, \tag{33}$$

where π_{mn}^{ref}, π_{mn}^{samp} and π_{mn}^{rest} denote the transition probability of reaching the state σ_n starting from σ_m within the state space of the reference, sampling and remaining distribution, respectively. Our algorithm now naturally follows from the above definitions. We can easily see that the microscopic reversibility condition in Eq. (31) is fulfilled, if we make use of a generator, which provides us configurations from $\rho^{\text{samp}}[\sigma]$. In addition, such an algorithm must satisfy the symmetric property of the stochastic matrix α^{rest}, so that $\rho^{\text{ref}}[\sigma]$ can finally be recovered by applying the Metropolis procedure regarding to $\rho^{\text{rest}}[\sigma]$. In summary, the following steps generate a configuration from $\rho^{\text{ref}}[\sigma]$:

Algorithm 1.

1. generate a uniform random variate, ξ, on $(0,1)$;
2. generate a configuration σ_n from the distribution $\rho^{\text{samp}}[\sigma]$;
3. perform Metropolis test with respect to $\rho^{\text{rest}}[\sigma]$, to check if σ_n is also part of the configuration space of $\rho^{\text{ref}}[\sigma] \rightarrow$ accept configuration with probability

$$\pi^{\text{rest}}_{A/mn} = \min\left(1, \frac{\rho^{\text{rest}}_n}{\rho^{\text{rest}}_m}\right); \tag{34}$$

4. if not go back to step (1).

We stress that an important aspect of this algorithm is to choose the appropriate sampling distribution $\rho^{\text{samp}}[\sigma]$, to extract meaningful results from the simulation. For this, the following points must be considered: (1) $\rho^{\text{samp}}[\sigma]$ should be free of zeroes in the whole configuration space, so that the ergodicity condition can be satisfied; (2) it should be a good approximation to the reference distribution $\rho^{\text{ref}}[\sigma]$, to enable an efficient importance sampling. This therefore also implies that the appropriate choice is strongly dependent on the external conditions imposed on the system. Now, supposing that for the sampling, we make use of the conventional procedure. Then, two possibilities naturally arise from the shape of the reference distribution. In order to introduce them, we redefine $\rho^{\text{ref}}[\sigma]$ in a factorized formulation

$$\rho^{\text{ref}}[\sigma] \propto \mathscr{G}[\sigma]\mathscr{H}[\sigma]\mathscr{Q}[\sigma] \tag{35}$$

with

$$\begin{aligned}
\mathscr{G}[\sigma] &= \exp\left[-\frac{1}{2\beta}\sum_{\vec{G}} \sigma^*(\vec{G})\Phi^{-1}(\vec{G})\sigma(\vec{G})\right], \\
\mathscr{H}[\sigma] &= \exp\left[\frac{\chi}{V}\int \exp\left[\psi(\vec{r})\right]\cos(\sigma(\vec{r}))\,\mathrm{d}\vec{r}\right], \\
\mathscr{Q}[\sigma] &= \left|\cos(\beta V^{\mathrm{I}/\mu VT}_{\text{eff}})\right|.
\end{aligned} \tag{36}$$

We see that an obvious simple way to calculate the functional averages in accordance with this factorization procedure is to generate configurations from the Gaussian distribution

$$\rho^{\text{samp}}[\sigma] \propto \mathscr{G}[\sigma], \tag{37}$$

employing, e.g., the Box–Müller method [33]. For this choice each configuration σ_n has equal probability to be chosen starting from state σ_m, since in the sequence all the states are independent of each other. Thus, in this case the symmetry condition of α^{rest}, $\alpha^{\text{rest}}_{mn} = \alpha^{\text{rest}}_{nm}$, is always satisfied. The reference distribution $\rho^{\text{ref}}[\sigma]$ is finally recovered by performing a Metropolis test with respect to the remaining distribution

$$\rho^{\text{rest}}[\sigma] \propto \mathscr{H}[\sigma]\mathscr{Q}[\sigma]. \tag{38}$$

However, this algorithm is not useful in the low temperature and/or large system size regime, because the acceptance probability of the Metropolis step becomes extremely small, which leads to unreliable results. In this range it is more judicious to perform the selection

$$\rho^{\text{samp}}[\sigma] \propto \mathscr{G}[\sigma]\mathscr{H}[\sigma] = \exp\left[-\beta V^{\mathrm{R}/\mu VT}_{\text{eff}}\right] \tag{39}$$

for the sampling distribution and

$$\rho^{\text{rest}}[\sigma] \propto \mathscr{Q}[\sigma] \tag{40}$$

for the remaining part, which provides an improved acceptance rate. Our procedure to generate configurations from this $\rho^{\text{samp}}[\sigma]$ relies on the concept of the HMC method of Duane et al. [22]. As we already

know from Section 3.2 this technique utilizes an MD algorithm to perform the multiple-move propagation. According to this strategy, we introduce a fictitious time τ and define the effective Hamiltonian

$$H_{\text{eff}}^{\text{samp}} = E_{\text{kin}} + V_{\text{eff}}^{\text{R}/\mu VT}, \tag{41}$$

where

$$E_{\text{kin}} = \frac{p_\sigma^2(\vec{G}=0)}{2m_\sigma(\vec{G}=0)} + \sum_{\vec{G}>0} \frac{p_\sigma^{\text{R}2}(\vec{G})}{2m_\sigma^{\text{R}}(\vec{G})} + \sum_{\vec{G}>0} \frac{p_\sigma^{\text{I}2}(\vec{G})}{2m_\sigma^{\text{I}}(\vec{G})} \tag{42}$$

represents the kinetic energy and $p_\sigma^{\text{R/I}}(\vec{G})$ the conjugate momentum of $\sigma^{\text{R/I}}(\vec{G})$ with $m_\sigma^{\text{R/I}}(\vec{G})$ as the corresponding field mass. In order to describe the evolution of the field degrees of freedom through phase space, we use Hamilton's equations of motion: [2]

$$\begin{aligned} \frac{\mathrm{d}\sigma^{\text{R/I}}(\vec{G})}{\mathrm{d}\tau} &= \frac{\partial H_{\text{eff}}^{\text{samp}}}{\partial p_\sigma^{\text{R/I}}(\vec{G})} = \frac{p_\sigma^{\text{R/I}}(\vec{G})}{m_\sigma^{\text{R/I}}(\vec{G})}, \\ \frac{dp_\sigma^{\text{R/I}}(\vec{G})}{\mathrm{d}\tau} &= -\frac{\partial H_{\text{eff}}^{\text{samp}}}{\partial \sigma^{\text{R/I}}(\vec{G})} = -\frac{\partial V_{\text{eff}}^{\text{R}/\mu VT}}{\partial \sigma^{\text{R/I}}(\vec{G})}, \end{aligned} \tag{43}$$

where the Hamiltonian $H_{\text{eff}}^{\text{samp}}$ is the constant of the motion. Now, to generate a Markov process with the limiting distribution $\rho^{\text{samp}}[\sigma]$, we apply the standard HMC algorithm as described in Section 3.2 and propagate the system through the corresponding phase space. For the numerical integration we use the Velocity Verlet integrator [11] which is time reversible. This property is a necessary requirement for the validity of the HMC method. The reference distribution $\rho^{\text{ref}}[\sigma]$ is finally recovered by performing a Metropolis test with respect to the remaining distribution $\rho^{\text{rest}}[\sigma]$, given in (40). The whole procedure is called the Metropolis auxiliary field hybrid Monte Carlo MS-AFHMC method. In order to definitely accept the HMC algorithm as a generator, we still have to convince ourselves that it satisfies the symmetry condition of α^{rest}. We can easily see that the algorithm fulfills this requirement by considering its validity proof in the original publication of Duane et al. [22].

Note that, in practice, we can choose the time step small enough, so that the acceptance step of the HMC algorithm is not necessarily needed. This is due to the fact that the ergodicity problem, caused by the logarithmic barriers, is here circumvented by generating configurations from a convenient sampling distribution $\rho^{\text{samp}}[\sigma]$. The resulting algorithm is then simply reduced to the massive stochastic collision algorithm of Andrea et al. with the constrain that the collisions must occur at the same time as the supplementary Metropolis step recovering $\rho^{\text{ref}}[\sigma]$. In the further development this procedure will be called the Metropolis auxiliary field hybrid molecular dynamics MS-AFHMD method.

3.3.2. The von Neumann procedure

The von Neumann procedure is based on the von Neumann rejection algorithm [11,31,34]. The strategy consists in splitting the reference distribution function $\rho^{\text{ref}}[\sigma]$ in a way as shown in Eq. (30), where now we assume that $\rho^{\text{samp}}[\sigma]$ is a distribution, from which it is easy to generate a configuration, and $\rho^{\text{rest}}[\sigma]$ a function which lies between zero and one. The following steps then generate a configuration from $\rho^{\text{ref}}[\sigma]$:

Algorithm 2.

1. generate a uniform random variate, ξ, on $(0,1)$;
2. generate a configuration σ_n from the distribution $\rho^{\text{samp}}[\sigma]$;

[2] The respective expressions for the gradients are given in Appendix A.

3. if $\xi \leqslant \rho^{\text{rest}}[\sigma_n]$ then σ_n is a configuration from $\rho^{\text{ref}}[\sigma]$;
4. if not go back to step (1).

In practice, we choose an algorithm to produce configurations from

$$\rho^{\text{samp}}[\sigma] \propto \mathscr{G}[\sigma]\mathscr{H}[\sigma] = \exp\left[-\beta V_{\text{eff}}^{\text{R}/\mu VT}\right] \tag{44}$$

and then perform the von Neumann rejection step with respect to

$$\rho^{\text{rest}}[\sigma] \propto \mathscr{Q}[\sigma]. \tag{45}$$

We stress that in the von Neumann procedure only the above factorization is possible, because $\rho^{\text{rest}}[\sigma]$ must be chosen between zero and one. To sample configurations from $\rho^{\text{samp}}[\sigma]$, we can again employ the HMC method or alternatively the massive stochastic collision method. Depending on the choice of the generator, the technique is called the von Neumann auxiliary field hybrid Monte Carlo VN-AFHMC or the von Neumann auxiliary field hybrid molecular dynamics VN-AFHMD method. Note finally that, as in the Metropolis procedure, we use the Velocity Verlet integrator for numerical integration and compute the gradient expressions given in Appendix A.

3.4. Selecting the field masses

Another important aspect to consider is the choice of the appropriate field masses. A simple selection procedure is to take one single value for all of them and estimate the error made in the numerical integration. The error estimation can be done by performing a microcanonical simulation and then evaluating the average deviation of the conserved quantity [35],

$$\Delta H_{\text{eff}}^{\text{samp}} = \frac{1}{\tau_{\text{run}}} \sum_{k=1}^{\tau_{\text{run}}} \left| \frac{H_{\text{eff}}^{\text{samp}}(k\Delta\tau) - H_{\text{eff}}^{\text{samp}}(0)}{H_{\text{eff}}^{\text{samp}}(0)} \right|, \tag{46}$$

where $\Delta\tau$ represents the time step of the simulation. However, what is not taken into account in this procedure is that each degree of freedom possesses a different width with respect to the sampling distribution $\rho^{\text{samp}}[\sigma]$, leading to an unequal speed of propagation through configuration space. In order to treat all the degrees of freedom equally, we have therefore devised a preconditioning scheme, which allows an individual adjustment of all the field masses. The procedure follows in spirit the AFMC method, where during the equilibration phase the maximum displacement of each degree of freedom is adjusted, to give a predefined acceptance rate. In practical application, the preconditioning is achieved in the so-called adjustment phase, in which the trajectory is propagated as under normal simulation conditions. However now, at intervals, the configurations are subjected to a Metropolis procedure and the masses are varied until the desired acceptance rate is obtained. Finally, all the masses are scaled through the largest one and multiplied with the predefined value. The largest mass is then taken as the reference. In Fig. 1 we show the masses of the field degrees of freedom as a function of the $\vec{\mathbf{G}}$-length determined during the adjustment phase of a preconditioned GC-MS-AFHMD simulation. In the calculation we considered a system of Gauss-core particles of a volume of $V_{\text{G}}^* = 20.0$ kept at a temperature of $T_{\text{G}}^* = 0.1$. The input value for the μ-dependent parameter χ has been estimated with the method of thermodynamic integration employing canonical molecular dynamics results of a system of 864 particles at a density of $\rho_{\text{G}}^* = 1.0$ [8–10]. We emphasize that the external parameters were chosen close to the limit of applicability of the GER method where the sign problem is already severe. The field cutoff was set to $E_{\text{cut/G}}^* = 40.0$, which corresponds to a total number of 81 degrees of freedom [36], and for the numerical integration a time step of $\Delta\tau_{\text{G}}^* = 0.01$ was chosen. By analyzing the plot, we see that the value of the masses continuously increase with increasing length of the

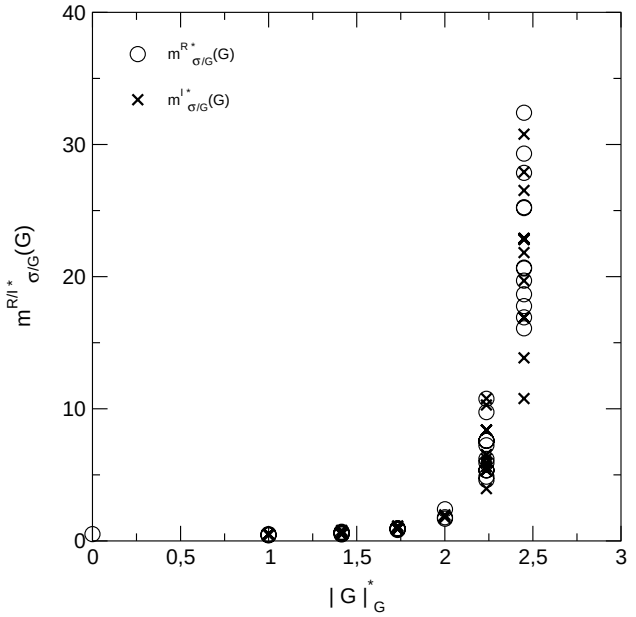

Fig. 1. Masses of the field degrees of freedom as a function of the $\vec{G}$-length determined during the adjustment phase of a preconditioned GC-MS-AFHMD simulation. In the calculation we considered a system of Gauss-core particles of a volume of $V^*_G = 20.0$ kept at a temperature of $T^*_G = 0.1$.

$\vec{G}$-vectors. The discrepancy between the maximum and minimum mass approximately amounts to $\Delta^*_{m_{\sigma/G}} \approx 32$. Moreover, we notice that the masses of the real and imaginary part of the field degrees of freedom show almost the same behavior, which is mainly caused by the influence of the Gaussian term in the effective potential. Finally, we can also deduce from this investigation that a preconditioned propagation should become more efficient with increasing number of degrees of freedom.

To test their usefulness in practical application, we have employed the single-mass and preconditioning scheme in the computation of a system of Gauss-core particles using the same simulation parameters as previously. To determine the optimal field masses, we have carried out several microcanonical auxiliary field calculations with the single-mass scheme utilizing different field masses and performed an additional calculation with the preconditioning scheme. In these simulations we have adjusted the average temperature to $\langle T^*_G \rangle_{NVE} = 0.1$. In Fig. 2 we give the results for the base 10 logarithm of the average deviation of the conserved quantity as a function of the field mass, computed with both strategies. Assuming that an error of $\log_{10} \Delta H^{\text{samp}}_{\text{eff}} = -4.5$ is common in practical application [37], we can conclude from the figure that a field mass of $m^*_{\sigma/G} = 8.1$ is an appropriate choice for the single-mass scheme and that no further Metropolis step is required to correct the discretization error. In case of the preconditioning scheme we have instead, approximately for the same accuracy, a set of field masses ranging from $m^*_{\sigma/G} \approx 0.4$ to 32.4. Therefore, we can safely predict that, if we make use of this technique in the simulation, the speed of evolution of the trajectory will be largely enhanced due to the smaller masses.

4. Results and discussion

In this section we demonstrate the validity and assess the efficiency of the auxiliary field algorithms previously discussed. In order to test whether they generate the correct average values, we applied them to

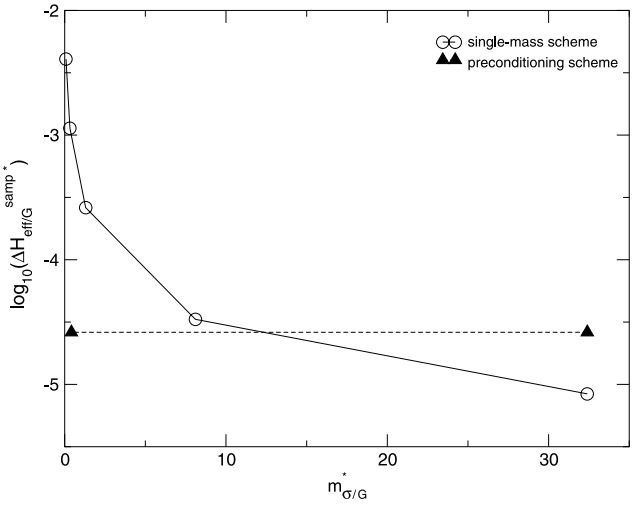

Fig. 2. Base 10 logarithm of the average deviation of the conserved quantity as a function of the field mass obtained from micro-canonical simulations, using the single-mass and preconditioning scheme. In the calculations we considered a system of Gauss-core particles of a volume of $V_G^* = 20.0$, adjusted to an average temperature of $\langle T_G^* \rangle_{NVE} = 0.1$.

the computation of a system of Gauss-core particles by employing the same simulation parameters as in the previous calculations. In Table 1 we show the values obtained for the average density and average potential energy per average particle number. For comparison, we give the result computed with the standard GCMC algorithm of Norman and Filinov [39]. In this calculation we simulated a system of Gauss-core particles of a box size of $V_G^* = 864.0$. First, we see that all the average quantities calculated with the AF-HMD algorithms are in good agreement with the values determined with the GCMC and GC-AFMC method. Moreover, we notice that even the run with the smaller field mass of $m_{\sigma/G}^* = 0.324$ provides good estimates for our thermodynamic properties.

Next, we regard the sampling efficiency of our multiple-move algorithms and assess their competitiveness with respect to the single-move GC-AFMC algorithm. For this, we consider two criteria, the statistical inefficiency and the CPU-time required, to generate a statistical independent configuration. The statistical inefficiency, defined as [11]

$$s = \lim_{\tau_{run} \to \infty} \frac{\tau_{run} \sigma^2(\langle \mathcal{O} \rangle_{run})}{\sigma^2(\mathcal{O})}, \tag{47}$$

Table 1
Average density and average potential energy per average particle number obtained for a system of Gauss-core particles of a volume of $V_G^* = 20.0$ kept at a temperature of $T_G^* = 0.1$ using different grand canonical simulation algorithms

Method	$m_{\sigma/G}^*$	$\langle \rho_G^* \rangle_{\mu VT}$	$\langle \Phi_G^* \rangle_{\mu VT} / \langle N \rangle_{\mu VT}$
GCMC	–	$0.997899 \pm 4.4E-05$	$2.34104 \pm 2.4E-04$
GC-MS-AFHMD	8.1	$0.9962 \pm 5.1E-03$	$2.347 \pm 1.2E-02$
GC-MS-AFHMD*	8.1	$1.000 \pm 1.5E-02$	$2.334 \pm 3.2E-02$
GC-MS-AFHMD*	0.324	$0.9981 \pm 3.5E-03$	$2.3477 \pm 8.9E-03$
GC-VN-AFHMD	8.1	$0.9983 \pm 4.4E-03$	$2.342 \pm 1.1E-02$
GC-AFMC	–	$0.9982 \pm 4.7E-03$	$2.341 \pm 1.1E-02$
prec. GC-MS-AFHMD	32.4	$0.9980 \pm 1.4E-03$	$2.3407 \pm 3.4E-03$

* Stochastic step every 10th MD-step, otherwise every 50th MD-step.

Table 2
Statistical inefficiencies of the sign function and the particle number numerator obtained for a system of Gauss-core particles of a volume of $V_G^* = 20.0$ kept at a temperature of $T_G^* = 0.1$ using different grand canonical auxiliary field algorithms

Method	$m_{\sigma/G}^*$	s_{sign}	$s_{signnum}$
GC-MS-AFHMD	8.1	17.5	14.0
GC-MS-AFHMD*	8.1	420	350
GC-MS-AFHMD*	0.324	17.6	12.5
GC-VN-AFHMD	8.1	18.2	15.3
GC-AFMC	–	260	220
prec. GC-MS-AFHMD	32.4	2.8	2.4

* Stochastic step every 10th MD-step, otherwise every 50th MD-step.

Table 3
CPU-times needed to generate a statistically independent configuration, obtained for a system of Gauss-core particles of a volume of $V_G^* = 20.0$ kept at a temperature of $T_G^* = 0.1$ using different grand canonical auxiliary field algorithms

Method	$m_{\sigma/G}^*$	t_{sign}^{CPU}	$t_{signnum}^{CPU}$
GC-MS-AFHMD	8.1	1.29	1.03
GC-MS-AFHMD*	8.1	6.99	5.83
GC-MS-AFHMD*	0.324	0.29	0.21
GC-VN-AFHMD	8.1	1.37	1.15
GC-AFMC	–	0.28	0.24
prec. GC-MS-AFHMD	32.4	0.21	0.18

* Stochastic step every 10th MD-step, otherwise every 50th MD-step.

determines the ability of the method in generating a new statistically independent configuration, which contributes to the running average of the functional $\mathcal{O}$, and therefore gives a measure how fast this average converges to its limiting value. As a general rule, we can say that the smaller this quantity the faster the statistical convergence. Since in case of the auxiliary field approach, we calculate the average of a physical quantity A through the ratio of two averages, i.e., $\langle \mathcal{A}\ \text{sign}\rangle/\langle \text{sign}\rangle$, we must regard their respective statistical inefficiencies. In Table 2 we give the inefficiencies of the sign function, s_{sign}, and the particle number numerator, $s_{signnum}$, obtained with different grand canonical auxiliary field algorithms. For the determination of these quantities we used the block averaging method [11,38]. By analyzing the results, we note that the preconditioned GC-MS-AFHMD algorithm produces by far the smallest statistical inefficiencies of all the AFHMD algorithms, while achieving at the same time a high accuracy in the numerical integration. Moreover, we deduce from the values, evaluated with the GC-MS-AFHMD algorithm using a field mass of $m_{\sigma/G}^* = 8.1$, that it is much more advantageous to perform a stochastic step at every 50th MD-step than at every 10th MD-step. This can be explained by the fact that the trajectory is less often perturbed which enables a faster propagation through phase space and consequently a faster generation of statistically independent configurations. Finally, we observe that choosing a Metropolis or a von Neumann procedure do not fundamentally influence the data correlation. Their respective statistical inefficiencies are almost equal with a slight advantage to the Metropolis approach.

The second important criterion is the computational cost required to generate a statistically independent configuration. In Table 3 we give the CPU-times t_{sign}^{CPU} and $t_{signnum}^{CPU}$ [3] needed to generate a statistically independent configuration for the sign function and the particle number numerator, respectively, obtained by employing different grand canonical auxiliary field algorithms. First, we note that the preconditioned GC-MS-AFHMD algorithm is again the most efficient of all the sampling methods and that the GC-AFMC

[3] Machine type: IBM RS/6000-43P-140; processor/clock-rate: PowerPC_604e/332 MHz.

algorithm is also very competitive taking the second place. The efficiency of the latter is almost comparable to the one of the GC-MS-AFHMD method, if a field mass of $m^*_{\sigma/G} = 0.324$ and a stochastic step frequency of $v_s = 10$ is used. Finally, by comparing the von Neumann and Metropolis GC-AFHMD results for the same simulation parameters, we see that the Metropolis procedure is more efficient in generating new configurations.

5. Summary and conclusions

In summary, we have presented in this paper two new classes of force-based algorithms conceived for an efficient computation within the auxiliary field methodology. They possess the major advantage over the standard single-move Metropolis Monte Carlo algorithm to permit multiple-move propagation allowing a faster diffusion through phase space. This is of particular importance, since the method suffers from a sign problem, which considerably deteriorates the convergence properties in the low temperature and/or large system size regime. The problem relates to the real and non-positive definite nature of the original distribution. To circumvent the difficulty, it is convenient to use the conventional procedure, which consists in factorizing the absolute value and including the remaining sign-function in the estimator. The resulting distribution possesses a discontinuous configuration space, which splits up into isolated regions separated by barriers of zero probability. In practical application, the sampling of such a distribution leads to a problem of ergodicity, if one wants to use a purely deterministic algorithm. The two algorithms we propose cross the barriers without difficulties and permit to maintain optimal convergence properties by generating configurations from the desired conventional distribution. The first one utilizes the hybrid Monte Carlo method in combination with a supplementary Metropolis step, while the second one makes use of the concept of the von Neumann rejection technique. They have in common that they both rely on a reweighting strategy and employ the molecular dynamics method, to perform the multiple-move propagation. Derived from these methods, we present in addition several variants, which slightly differ in their suitability for practical application. Moreover, we further optimize the sampling by taking into account that each degree of freedom possesses a different width with respect to the sampling distribution. This leads to an unequal speed of propagation, if one utilizes only a single fictive mass to perform the Newtonian dynamics. In this work we present a preconditioning scheme, which allows to treat all the degrees of freedom on an equal footing by adjusting each mass independently. To assess the competitiveness of these auxiliary field algorithms, we perform calculations on a system of Gauss-core particles. We find that a variant of the supplemented hybrid Monte Carlo method in combination with the preconditioning scheme is by far the most efficient algorithm in generating statistical independent configurations per computational cost and enables a numerical integration of high accuracy. The single-mass algorithms can instead be made as fast as the standard Metropolis Monte Carlo method, while keeping the discretization error acceptably small. We can safely predict that with increasing resolution the benefit of the multiple-move algorithms adopting the preconditioning scheme will considerably grow with regard to the other ones, because the preconditioning takes care of the fact that the displacements of the coefficients with larger $\vec{G}$-length do not significantly contribute to the evolution of the system.

To conclude, we point out that all the capabilities of the algorithms presented in this work are yet by far not exhausted and we hope that they may also be useful for other methods dealing with a complex or non-positive definite Boltzmann-factor.

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Appendix A. Forces on the auxiliary field degrees of freedom

In this section we give the set of first-order derivatives of the effective potential with respect to the auxiliary field degrees of freedom:

$$\frac{\partial V_{\mathrm{eff}}^{\mathrm{R}/\mu VT}}{\partial \sigma(\vec{G}=0)} = \frac{\sigma(\vec{G}=0)}{\beta^2 \Phi(\vec{G}=0)} + \frac{\chi}{\beta V}\int \exp\left[\psi(\vec{r})\right]\sin(\sigma(\vec{r}))\,\mathrm{d}\vec{r},$$

$$\frac{\partial V_{\mathrm{eff}}^{\mathrm{R}/\mu VT}}{\partial \sigma^{\mathrm{R}}(\vec{G})} = \frac{2\sigma^{\mathrm{R}}(\vec{G})}{\beta^2 \Phi(\vec{G})} + \frac{2\chi}{\beta V}\int \exp\left[\psi(\vec{r})\right]\sin(\sigma(\vec{r}))\cos(\vec{G}\vec{r})\,\mathrm{d}\vec{r}, \tag{A.1}$$

$$\frac{\partial V_{\mathrm{eff}}^{\mathrm{R}/\mu VT}}{\partial \sigma^{\mathrm{I}}(\vec{G})} = \frac{2\sigma^{\mathrm{I}}(\vec{G})}{\beta^2 \Phi(\vec{G})} - \frac{2\chi}{\beta V}\int \exp[\psi(\vec{r})]\sin(\sigma(\vec{r}))\sin(\vec{G}\vec{r})\,\mathrm{d}\vec{r}.$$

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