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Finite population-size effects in projection Monte Carlo methods

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Abstract

Projection (Green's function and diffusion) Monte Carlo techniques sample a wave function by a stochastic iterative procedure. We show that these methods converge to a stationary distribution which is unexpectedly biased, i.e., differs from the exact ground state wave function, and that this bias occurs because of the introduction of a replication procedure. We demonstrate that these biased Monte Carlo algorithms lead to a modified effective mass which is equal to the desired mass only in the limit of an infinite population of walkers. In general, the bias scales as $1/N$ for a population of walkers of size N. Finally, we consider various strategies to reduce this bias.

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1 Introduction

In the last two decades, Monte Carlo (MC) methods have been widely employed for studying quantum mechanical problems (see [1] for a recent review). In particular, they have proven to be valuable in determining ground state properties of particle [2, 3, 4], nuclear [5, 6, 7], atomic [8], and molecular systems [9], as well as of quantum fluids and solids [10, 11, 12, 13].

Projection MC methods, which are our concern here, attempt to project out the ground state of a quantum system. The various alternative implementations correspond to different choices of the projection operator. Among the many MC methods which have been developed, it is convenient to distinguish two main classes: Green's Function Monte Carlo (GFMC) methods, which essentially use the Green's function H^{-1} as a projector, and diffusion Monte Carlo (DMC) methods which use the imaginary time evolution operator $\exp(-Ht)$ as a projector. These methods are best understood as stochastic implementations of the power method. In that method, the dominant eigenvalue and eigenvector of a matrix or projection operator A is computed by iteratively applying A on an arbitrary initial vector $|\phi\rangle$ [14]. As the number of iterations n becomes large, one has

$$A^n|\phi\rangle = \lambda_0^n \langle\psi_0|\phi\rangle|\psi_0\rangle + \mathcal{O}({\lambda_1}^n) \tag{1}$$

where λ_0 is the leading eigenvalue, ψ_0 is the corresponding eigenvector, and λ_1 is the largest sub-leading eigenvalue. Then one has [14, 15]

$$\lambda_0 = \lim_{n\to\infty} \left(\frac{||A^{n+k}|\phi\rangle||}{||A^n|\phi\rangle||} \right)^{1/k} \tag{2}$$

for any integer k.

To implement this method stochastically, one first defines a matrix M_{ij} such that each column sums to one (to ensure probability normalization), $\sum_i M_{ij} = 1$. The matrix A is then expressed as a product of the matrix M and a diagonal matrix w,

$$A_{ij} = M_{ij} w_j \ , \qquad \text{with } w_j = \sum_i A_{ij} \ . \tag{3}$$

The matrix M defines a Markov process which is used to generate the sequence of states (called configurations hereafter): given the configuration j, configuration i is chosen with probability M_{ij}. The matrix w makes it necessary to weight the configurations so that during evolution, the weight associated with configuration j is multiplied by w_j. It is easy to show that on average the evolution is identical to the standard power method (i.e., without stochasticity), so that equation (1) is reproduced for mean values. Thus the configurations after a large number n of steps will form a sample of the dominant eigenvector. If the population consists of N random walkers ($\alpha = 1, \cdots, N$) in configurations i_α, carrying the weight w_α, then

$$F(i) = \sum_{\alpha=1}^{N} \delta_{i,i_\alpha} w_\alpha \tag{4}$$

is an estimator of the ith component of the (unnormalized) dominant eigenvector of A in the limit of many iterations. The number of iterations should be chosen large enough so that sub-dominant eigenvectors are projected out. However, in practice, this method of carrying weights does not work well because the variance of the above estimator grows exponentially with the number of iterations while it decreases only with the usual $1/N$ law. There are several possibilities to remedy this problem. One is to repeat the n iterations a large number of times (see e.g. [16]) using R independent runs (but still using the same initial vector ϕ). The variance of any estimator will diminish as $N^{-1}R^{-1}$ since the walkers are all independent. This relatively slow decrease will have to compensate a variance which is exponentially large in n. Another way to remedy the problem is to reduce the variance; this can be achieved by "replicating" the population of walkers [17]. The idea here is to discard low weight configurations and duplicate large weight configurations. This replication does not change the fact that the number $N^{(n)}$ of configurations at iteration n (or their total weight) either increases or decreases exponentially with n because of the λ_0^n factor. To avoid this, it would be best to evolve with the projection operator A/λ_0, but of course λ_0 is not known. So in practice, one uses a population control method whereby the random walkers are evolved using $A/\lambda(n)$ and then replicated, where at each step $\lambda(n)$ is adjusted to keep the population size or its total weight approximately constant. It has become common usage in this field to call "replication" the *combination* of this population control and the application of the above replication procedure, so that we will follow this nomenclature in the rest of the paper.

The above evolution followed by replication (i.e., replication *and* population control) forms a Markov chain in the space of populations of weighted configurations, and thus has a stationary probability distribution ψ^*. It is standard procedure to consider that ψ^* gives configurations distributed according to the ground state wave function. However, this is not justified; in fact, ψ^* is *not* a multiple of ψ_0, rather ψ^* is a biased estimator of ψ_0. The amplitude of the bias goes to zero as $1/N$ where N is the characteristic size of the population used in the iterations. This bias is generic to any replication (population control) method and occurs as soon as the w matrix is not a multiple of the identity matrix. A qualitative way of arguing for the existence of such a bias is obtained by considering the case of a single random walker ($N = 1$). In this case, the replication procedure will amount to forgetting the weight after each replication (e.g., the weight is reset to one). The diffusion thus proceeds according to the transition probabilities M_{ij} only, and the corresponding limit distribution clearly differs from the desired eigenvector ψ_0 of A. It is reasonable to assume that this bias remains for other values of N, and that it goes to 0 as $N \to \infty$, since the procedure is equivalent to the non-stochastic case in that limit.

The existence of a bias for the eigenvalue estimator was first noticed by Kalos [18] and by Ceperley and Kalos [19]; it was rediscovered by Nightinghale and Blöte [20] for transfer matrix calculations, as well as by Gelbard [21] in the context of neutronics computations. However, it was Hetherington [22] who first explicitly stated that ψ^* was biased by order $1/N$ at least for his particular choice of replication procedure. Nevertheless, it was not explicitly recognized that the bias is intrinsically related to replication, as will be shown below. In spite of these (few) papers, in most works using projection Monte Carlo, it is not realized that ψ^* is biased,

or at best the bias is believed to be negligible. The aim of the present paper is to demonstrate the existence of this finite population-size bias in a general case, to estimate its magnitude as well as its scaling, and to consider ways to correct it.

Our discussion of the bias applies to GFMC, to DMC, and also to all stochastic implementations of the power method. In particular, it applies to MC calculations for transfer matrices in statistical mechanics. However, we will present most of the derivations for DMC. The advantage is that it can be interpreted in terms of Feynman path integrals which renders the discussion easier for our purposes. After briefly reviewing GFMC and DMC in Section 2, we calculate in Section 3 the errors introduced by a particular choice of the replication. Section 4 illustrates the bias on a pairing Hamiltonian, showing that it can be rather important. Finally, we review different strategies that can be used or have been proposed to reduce this bias (Section 5).

2 Projection Monte Carlo methods

2.1 Green's function Monte Carlo

The GFMC method was first developed by Kalos and coworkers [23, 18, 10], providing a technique for calculating the ground state energy of a quantum system using random walks. In order to be explicit, we will present the case of a point $\mathbf{r}$ in configuration space placed in the potential $V(\mathbf{r})$. The time-independent Schrödinger equation (with $\hbar \equiv 1$) is

$$\left[-\frac{1}{2m}\nabla^2 + V(\mathbf{r}) - E_S\right]\psi(\mathbf{r}) = (E_0 - E_S)\psi(\mathbf{r}) \tag{5}$$

where E_0 is the ground state energy, and E_S is arbitrary for the moment. This equation can be transformed into an integral equation by use of the Green's function $G(\mathbf{r},\mathbf{r}')$ of the operator on the left side of equation (5), solution of

$$\left[-\frac{1}{2m}\nabla^2 + V(\mathbf{r}) - E_S\right]G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \tag{6}$$

The additional energy shift E_S is to be chosen so that $G(\mathbf{r},\mathbf{r}')$ is positive (see below). Substitution in (5) gives the Fredholm integral equation

$$\psi(\mathbf{r}) = (E_0 - E_S)\int G(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')\,d\mathbf{r}' \tag{7}$$

which can be solved by iteratively applying the relation

$$\psi^{(n+1)}(\mathbf{r}) = (E_0 - E_S)\int G(\mathbf{r},\mathbf{r}')\psi^{(n)}(\mathbf{r}')\,d\mathbf{r}'. \tag{8}$$

Thus $\psi^{(n)}$ tends asymptotically to a multiple of the ground state wave function ψ_0. In practice, these iterations are followed stochastically by use of a MC method, i.e. by sampling the successive $\psi^{(n)}$'s by a population of random walkers. Starting from a set of configurations $\{\mathbf{r}^{(n)}\}$

selected at random from the density distribution $\psi^{(n)}(\mathbf{r})$, a new set $\{\mathbf{r}^{(n+1)}\}$ is obtained by moving each configuration $\mathbf{r}^{(n)}$ to $\mathbf{r}^{(n+1)}$ according to the probability function $(E_0 - E_S)G(\mathbf{r}^{(n+1)}, \mathbf{r}^{(n)})$ conditional on $\mathbf{r}^{(n)}$. The main technical difficulty consists in treating the propagator, which is unknown in general. The GFMC method necessitates thus a second step, which is the sampling of the Green's function by an additional Neumann-Ulam random walk [10, 19]. Note that the energy shift must be chosen so that $E_S < E_0$, in order to have a positive propagator (to allow for the MC implementation). Of course, the exact energy E_0 of the ground state which enters into the propagator is unknown in advance (we are seeking for it). However, it is clear that, if E_0 is replaced by a trial energy E_T in equation (8), the successive iterations will still tend to a multiple of ψ_0. If E_T is larger than E_0, the $\psi^{(n)}$'s will grow in normalization (resulting in a growth in the population of walkers), whereas the contrary occurs for E_T smaller than E_0. In fact, E_T is adjusted during the MC run in order to maintain an approximately constant population size.

In summary, with GFMC methods, the resolvent operator $(E_T - E_S)/(H - E_S)$ is used to filter out the ground state $|\psi_0\rangle$ from an initial trial wave function $|\psi_T\rangle$:

$$|\psi_0\rangle \propto \lim_{n\to\infty} \left(\frac{E_T - E_S}{H - E_S}\right)^n |\psi_T\rangle \tag{9}$$

The change in population size can be used to estimate the energy E_0 of the ground state. Indeed, the normalization – or growth – estimator is written as

$$E_N = E_S + (E_T - E_S)\frac{N^{(n)}}{N^{(n+1)}} \tag{10}$$

with $N^{(n)}$ being the number of walkers at the n-th iteration. As noted first in ref. [18], this estimator is biased even after relaxation (when the limit distribution is attained) as a consequence of the statistical fluctuations of the $N^{(n)}$'s. Another estimator of E_0 can be constructed by use of the expression

$$E_0 = \frac{\langle\psi_0|H|\psi_T\rangle}{\langle\psi_0|\psi_T\rangle} \tag{11}$$

It is possible to guide the random walk in order to improve the sampling. Consider the density function $\rho(\mathbf{r}) \equiv \psi(\mathbf{r})\psi_T(\mathbf{r})$ with $\psi_T(\mathbf{r})$ being time independent. It obeys the iterative equation obtained from eq. (8):

$$\rho^{(n+1)}(\mathbf{r}) = (E_T - E_S)\int \left[\psi_T(\mathbf{r})G(\mathbf{r},\mathbf{r}')\psi_T^{-1}(\mathbf{r}')\right]\rho^{(n)}(\mathbf{r}')\, d\mathbf{r}' \tag{12}$$

With the standard (non-stochastic) iterative method (called the power method in the case of matrices), this function $\rho(\mathbf{r})$ converges to $\psi_0(\mathbf{r})\psi_T(\mathbf{r})$, and thus one can write a trial estimator (also called mixed, or variational estimator) of E_0 as

$$E_T = \frac{\langle\rho\psi_T^{-1}|H|\psi_T\rangle}{\langle\rho\psi_T^{-1}|\psi_T\rangle} = \frac{1}{N}\sum_{k=1}^{N}\psi_T^{-1}(\mathbf{r}_k)\left[-\nabla^2 + V(\mathbf{r}_k)\right]\psi_T(\mathbf{r}_k) \tag{13}$$

where $N \equiv N^{(n)}$ is the population size at time n, and the $\mathbf{r}_k \equiv \mathbf{r}_k^{(n)}$ are the configurations of the N points. Note that, in practice, this estimator is averaged along the MC run. Thus, one can say from eq. (12) that the random walk is guided by the trial wave function ψ_T in order to importance sample the solution ψ_0. The configuration space is explored by the random walk with a density distribution given by the guiding wave function ψ_T. If this (arbitrary) function is chosen close to the exact ψ_0 using *a priori* knowledge of the solution, the variance on this estimator will be significantly smaller. This allows one to gain higher accuracy through variance reduction. (In fact, it is evident that the variance vanishes in the limit $\psi_T \to \psi_0$). In the case where we put $\psi_T \equiv 1$, the iteration equation (12) comes back to eq. (8), so that the random walk is unguided. Then, the trial energy estimator becomes simply

$$E_T = \frac{1}{N}\sum_{k=1}^{N} V(\mathbf{r}_k) \tag{14}$$

Note that the unguided random walk asymptotically samples ψ_0, whereas the guided one samples the physical probability distribution $|\psi_0|^2$ (to the extent to which ψ_T is a good approximation of ψ_0).

2.2 Diffusion Monte Carlo

We now briefly present the DMC method [17]. The first step is to note the similarity between the time-dependent Schrödinger equation and a reaction-diffusion equation. Indeed, the Schrödinger equation in imaginary time (with $\hbar \equiv 1$) reads

$$\frac{\partial\psi}{\partial t} = -H\psi = \frac{1}{2m}\nabla^2\psi(\mathbf{r},t) - V(\mathbf{r})\psi(\mathbf{r},t) \tag{15}$$

so that the right-hand side can be interpreted as a diffusion term (with a diffusion constant $D = 1/2m$) and a reaction term (with a source-sink term of the form $-V\psi$). As it is well known, the diffusion can be treated via a random walk, whereas the reaction equation, in the absence of diffusion, describes a simple growth or decay process. This coexistence of a diffusion and a growth/decay process will be important in the following.

The imaginary time evolution given by equation (15) acts as a projector which, at large time, selects out the lowest energy state. In order for the ground state to survive the exponential decay, it is appropriate to shift the potential by E_0, thus giving

$$\frac{\partial\psi}{\partial t} = (E_0 - H)\psi = \frac{1}{2m}\nabla^2\psi(\mathbf{r},t) - (V(\mathbf{r}) - E_0)\psi(\mathbf{r},t) \tag{16}$$

The projector in this method is thus the (imaginary) time evolution operator $U_t = \mathrm{e}^{-(H-E_0)t}$. In order to evaluate U_t in practice, it is necessary to resort to the short time approximation. First divide the time interval t into M infinitesimal intervals Δt, and use the relation

$$U_t = \prod_{n=1}^{M} \mathrm{e}^{-(H-E_0)\Delta t}. \tag{17}$$

The infinitesimal propagators are then approximated by use of a breakup such as

$$e^{-(H-E_0)\Delta t} = e^{-T\Delta t} e^{-(V-E_0)\Delta t} + \mathcal{O}(\Delta t^2) \tag{18}$$

where T and V stand for the kinetic and potential energy, respectively. (It is of course possible to use breakups which are more accurate.) Applying the evolution operator on an initial trial wave function ψ_T yields for large t

$$\psi_0(\mathbf{r}) \simeq \int d\mathbf{r}^{(M)} \cdots d\mathbf{r}^{(0)} \, \langle \mathbf{r}|e^{-\Delta t T}|\mathbf{r}^{(M)}\rangle e^{-\Delta t(V(\mathbf{r}^{(M)})-E_0)} \\ \cdots \langle \mathbf{r}^{(1)}|e^{-\Delta t T}|\mathbf{r}^{(0)}\rangle e^{-\Delta t(V(\mathbf{r}^{(0)})-E_0)} \psi_T(\mathbf{r}^{(0)}). \tag{19}$$

We have assumed that the potential $V(\mathbf{r})$ is local in configuration space, so that applying $e^{-\Delta t(V-E_0)}$ simply amounts to multiplying by a weight. The operator $e^{-\Delta t T}$ corresponds to a diffusion operator whose matrix elements are

$$P(\mathbf{r}', \mathbf{r}) \equiv \langle \mathbf{r}'|e^{-\Delta t T}|\mathbf{r}\rangle = \left(\frac{m}{2\pi\Delta t}\right)^{d/2} \exp\left(-\frac{m}{2\Delta t}(\mathbf{r}-\mathbf{r}')^2\right) \tag{20}$$

where d stands for the dimension of the problem. The application of the operator P can be simulated by MC, through a random step drawn from a (d-dimensional) gaussian distribution of variance $\Delta t/m$. Finally, the repeated iteration of $e^{-(H-E_0)\Delta t}$ can be simulated using an ensemble of (weighted) random walkers, similarly to what is done in GFMC. At each iteration, a random walker at $\mathbf{r}$ is weighted by a factor $w(\mathbf{r}) = e^{-\Delta t(V(\mathbf{r})-E_0)}$, and then diffused according to a gaussian step. This is analogous to the Feynman separation of the time-evolution operator into two separate propagators (corresponding to the potential and the kinetic energy) [24]. Here, the kinetic energy T tends to spread out the wave function in configuration space (diffusion), whereas the potential energy V concentrates the wave function in its components with low $V(\mathbf{r})$ (reaction term). As in GFMC, the exact energy E_0 is not known in advance so it must be replaced by a trial energy E_T in the above formulae. The projection operator is thus $e^{-(H-E_T)\Delta t}$, and one has

$$|\psi_0\rangle \propto \lim_{n\to\infty} \left(e^{-(H-E_T)\Delta t}\right)^n |\psi_T\rangle \, . \tag{21}$$

This trial energy E_T is constantly adjusted along the random walk in order to avoid either an exponential increase or decrease in the total weight of the population. We can also define a normalization (or growth) estimator for the ground state energy:

$$E_N = -\frac{1}{\Delta t} \log\left(\frac{N^{(n+1)}}{N^{(n)}}\right) \tag{22}$$

Following the same reasoning as in the GFMC, a trial estimator of E_0 can be obtained by modifying the diffusion procedure in order to sample $\rho(\mathbf{r}) \equiv \psi(\mathbf{r})\psi_T(\mathbf{r})$, that is using the propagator $\psi_T(\mathbf{r})e^{-(H-E_T)\Delta t}\psi_T^{-1}(\mathbf{r})$. It can be shown that this propagator can be simulated by a diffusion in an external drift velocity field (function of $\nabla\psi_T(\mathbf{r})$), with a modified weight factor

$w(\mathbf{r}) = e^{-\Delta t(\psi_T^{-1}(\mathbf{r})H\psi_T(\mathbf{r})-E_T)}$. Then, the trial energy estimator takes the same form as eq. (13), and is thus less fluctuating than when taking $\psi_T(\mathbf{r}) \equiv 1$ (i.e., unguided random walk). In the following sections, we will restrict the discussion to the unguided case for simplicity, but our results can easily be extended to the guided case.

3 Systematic error due to replication

Now, we come to the critical point of the projection MC algorithms. If we follow the N random walkers, accumulating the weights through successive iterations, the variance on these weights increases exponentially. Since it is necessary to follow a large number of steps to project out the ground state, this approach is impracticable. Thus, to be efficient, the algorithm must discard walkers with small weights and duplicate those with large weights. This is the "replication" step, and we will demonstrate that it is the root of the bias in these algorithms.

One simple way to replicate is to sample a new population of walkers at each iteration according to the weights considered as a probability distribution, as proposed by Hetherington. However, this method is unnecessarily noisy, and leads to unefficient strong correlations among the walkers. This will be discussed later on. Among workers in the field, two major replications are used. The first one (see e.g. [9, 18, 23, 17, 25]) consists in considering the fractional part of the weights as a probability in order to deal with walkers of unit weight only. For each walker of weight w, one creates $\mathrm{int}(w + \xi)$ walkers of unit weight, where ξ is a random number uniformly distributed in $[0, 1]$. This replication procedure still introduces correlation among the walkers. An alternative approach has been proposed in ref. [20] in order to improve upon this. Each walker with a big weight (e.g. larger than 2) is replaced by two identical new walkers, each with weight equal to half of the old weight. Alternatively, two walkers with low weights w_a, w_b (e.g. smaller than 1/2) are combined to give one walker of weight $w = w_a + w_b$ which replaces the first or the second one with probabilities proportional to the weights w_a and w_b. The remaining walkers are unchanged by the replication (i.e., they keep their weights). That algorithm reduces the unnecessary random fluctuation of the total weight of the walkers during replication.

As noted in ref. [18, 19, 20, 26], both energy estimators are inherently biased. In fact, all simple-minded estimators (c.f. Section 5.4) will be biased because there is a bias on the wave function itself $\psi(\mathbf{r})$ which survives asymptotically, even when the trivial bias due to the initial condition ($\psi_T \neq \psi_0$) has dissapeared (i.e., after relaxation). This failure to sample the exact probability distribution (i.e., the ground state wave function or its square) originates from the necessity to normalize the weights at some point in the algorithm. Thus, the replication process is the fundamental reason for the existence of a bias. One can understand this systematic error from different points of vue. One can say that the MC estimator for any observable always expresses as a ratio, whose numerator and denominator fluctuates. The correlation between the numerator and the denominator is then suggestive that there is a bias. Alternatively, one can regard the feedback of the number of walkers (or the total weight) into E_T (which is adjusted

along the random walk) as the origin of the bias, called therefore the population control bias in ref. [26]. In Section 3.1, we propose a simple model to understand how the replication produces a bias, and to estimate this bias.

In DMC, there is usually a residual time-step error (due to the breakup of the propagator). Thus, the entire walk is traditionally repeated with different Δt's, in order to extrapolate to the $\Delta t = 0$ limit. In GFMC on the contrary, the random process is supposed to tend to the exact ground state, at the cost of a more complex algorithm. However, since the effective time steps of the GFMC are very small, it has been argued that DMC is more efficient computationally [26]. In view of this, we will consider only DMC in the following. We will show that the finite size of the population of random walkers introduces a bias in the method. However, all the conclusions we draw are valid for GFMC, since the same population control (replication) is needed in order to keep the variance bounded.

3.1 Calculation of the bias in a simple model

For the sake of simplicity, we treat the case of a particle in a one-dimensional potential governed by the Hamiltonian $H = p^2/2m + V(x)$. This example illustrates simply the origin of the bias, but our results are easily extended to the general case (e.g. multi-dimensional potential, problems in other representations or basis sets). We follow the time evolution with replication of an ensemble of N points $\{x_i\}$ chosen from an arbitrary initial distribution $\psi(x)$. Our aim is to show that the evolved distribution will asymptotically tend to a wave function which is *not* the ground state solution $\psi_0(x)$ of the time-independent Schrödinger equation

$$-\frac{1}{2m}\psi_0'' + (V(x) - E_0)\psi_0(x) = 0 \tag{23}$$

where E_0 is the ground state energy. We take the wave function (*not* its square) to be a probability distribution, so that $\int \psi(x)\, dx = 1$. We evolve the N points using the infinitesimal imaginary time evolution operator. Its matrix elements (with $\hbar \equiv 1$, and $E_T \equiv 0$) are given by

$$U_{\Delta t}(x', x) = \langle x'|e^{-\Delta t\ H}|x\rangle = P(x', x)w(x) + \mathcal{O}(\Delta t^2) \tag{24}$$

where $w(x) = e^{-\Delta t\ V(x)}$ is the weight associated to the point x, and $P(x', x)$ is a gaussian distribution in x' with mean x and variance $\Delta t/m$. Note that the normalization condition for the probability distribution $P(x', x)$ imposes that $w(x) = \int U_{\Delta t}(x', x)\, dx'$, implying that both $w(x)$ and $P(x', x)$ have always an implicit dependence on Δt, for any choice of breakup of H. After evolution by Δt, we replicate in the following way. For each realization (i.e. N walkers at given positions), we normalize the weights after evolution in order to yield a discrete probability distribution for the position after evolution. Then we average over all the possible realizations (according to the initial wave function), thus giving a continuous probability distribution which gives the wave function after evolution. This leads to an evolution equation for the wave function as a function of imaginary time.

In the following, we will apply estimators acting on both the initial ensemble of points $\{x_i\}$ and the corresponding ensemble of points $\{x_i'\}$ after the evolution for a time Δt. Consider the random variables

$$W = \frac{1}{N}\sum_{i=1}^{N} w(x_i) \tag{25}$$

$$F(\tilde{x}) = \frac{1}{N}\sum_{i=1}^{N} w(x_i)\delta(\tilde{x} - x_i') \tag{26}$$

W is an estimator for the average weight of the population of points after time evolution, from which the standard normalization (or growth) estimate for the energy E_0 can be deduced:

$$E_N = -\frac{1}{\Delta t}\log(E[W]) \tag{27}$$

where $E[]$ denotes the expectation value. Also, the random variable $F_N(\tilde{x}) = F(\tilde{x})/W$ is an estimator of the *normalized* wave function $\tilde{\psi}(\tilde{x})$ after time evolution, that is

$$\tilde{\psi}(\tilde{x}) = E[F_N(\tilde{x})] \tag{28}$$

with obviously $\int \tilde{\psi}(\tilde{x})\, d\tilde{x} = 1$.

We are thus interested in determining the expectation value of both estimators W and F_N. As we are only concerned with the $\Delta t \to 0$ limit, the calculation is carried out by expanding $E[W]$ and $E[F_N]$ in powers of Δt, keeping only the leading terms. This is done in Appendix A. There we show that this calculation requires the determination of the covariance $\mathrm{Cov}[F, W]$. Note that the points x_i are independent in this simple model, leading to a feasable calculation of this covariance. For other replication procedures than the one used here, the x_i will not stay independent, and it is not possible to calculate exactly the steady state. The drawback of our choice of replication however is it is not readily implemented in practice. The end result is that in more general cases, the correlations induced by the replication process modify the steady state from the calculated one, but the scaling in N remains the same. Note that the degree of correlation is dependent on the details of the replication algorithm.

Finally, as shown in Appendix A, the distribution of $\tilde{x}$ after time evolution for Δt can be written as

$$\begin{aligned}\tilde{\psi}(\tilde{x}) = E[F_N(\tilde{x})] = \psi(\tilde{x}) &+ \frac{\Delta t}{2m}\psi''(\tilde{x}) \\ &-\Delta t\,(V(\tilde{x}) - E_0)\psi(\tilde{x}) + \Delta t\,\psi(\tilde{x})\int dx\,\psi(x)(V(x) - E_0) \\ &+\frac{\Delta t}{N}(V(\tilde{x}) - E_0)\psi(\tilde{x}) - \frac{\Delta t}{N}\psi(\tilde{x})\int dx\,\psi(x)(V(x) - E_0) + \mathcal{O}(\Delta t^2)\end{aligned} \tag{29}$$

Letting Δt tend to zero, one obtains

$$\frac{\partial\psi(\tilde{x}, t)}{\partial t} = \lim_{\Delta t \to 0}\frac{\tilde{\psi}(\tilde{x}) - \psi(\tilde{x})}{\Delta t}$$

$$
\begin{aligned}
&= \frac{1}{2m}\psi''(\tilde{x}) - (1-\frac{1}{N})(V(\tilde{x}) - E_0)\psi(\tilde{x}) \\
&\quad +(1-\frac{1}{N})\psi(\tilde{x})\int dx\ (V(x) - E_0)\psi(x)
\end{aligned} \tag{30}
$$

which yields a modified version of the Schrödinger equation in imaginary time, with an unusual third term on the right-hand side. Note also that the energies are scaled by a factor $(1-1/N)$ which tends to one for an infinite size sample. The correction in $1/N$ is due to the second term in the right-hand side of equation (58), and thus originates from the correlation between the numerator and the denominator in the expression of the normalized wave function.

Note that, by integrating over x the standard time-independent Schrödinger equation (23) for the ground state, one gets the expression

$$
E_0 = \int dx\ V(x)\psi_0(x)\ , \tag{31}
$$

where E_0 is the *true* (i.e., with $N \to \infty$) ground state energy and $\psi_0(x)$ is the exact ground state wave function. Note that this expression corresponds to our trial function estimate for the ground state energy E_0. As a consequence of (31), $\psi_0(x)$ is also the solution of the equation

$$
-\frac{1}{2m}\psi_0'' + (V(x) - E_0)\psi_0(x) - \psi_0(x)\int dx\ (V(x) - E_0)\psi_0(x) = 0 \tag{32}
$$

It is easy to show that the third term in (32) can be obtained by considering the evolution of

$$
\psi_0(x) = \frac{\phi(x)}{\int \phi(x)\ dx} \tag{33}
$$

where $\phi(x)$ is an *unnormalized* wave function which evolves according to the imaginary time Schrödinger equation

$$
\frac{\partial\phi}{\partial t} = \frac{1}{2m}\phi'' - (V(x) - E_0)\phi(x) \tag{34}
$$

One finds, using (34),

$$
\begin{aligned}
\frac{\partial\psi}{\partial t} &= \frac{\frac{\partial\phi}{\partial t} - \psi(x)\int\frac{\partial\phi}{\partial t}\ dx}{\int\phi(x)\ dx} \\
&= \frac{1}{2m}\psi'' - (V(x) - E_0)\psi(x) + \psi(x)\int(V(x) - E_0)\psi(x)\ dx\ ,
\end{aligned} \tag{35}
$$

which has as an asymptotic solution $\psi_0(x)$ given by equ. (32). Thus, our evolution equation (30) keeps the norm of $\psi(x)$ constant, and the third term in the right-hand side of (30) is simply equivalent to that in eq. (32) except for the factor $(1-1/N)$.

Now we are searching for the steady-state distribution $\psi^*(x)$ of our stochastic procedure, that is the stationary solution of eq. (30):

$$
-\frac{1}{2m^*}\psi^{*\prime\prime} + (V(x) - E_0)\psi^*(x) - \psi^*(x)\int dx\ (V(x) - E_0)\psi^*(x) = 0 \tag{36}
$$

Thus, because of the sampling procedure, we have to deal with an effective mass m^* defined as

$$m^* = m\left(1 - \frac{1}{N}\right) \tag{37}$$

If $\psi^*(x)$ is taken as the solution of the standard Schrödinger equation for a particle of mass m^*,

$$-\frac{1}{2m^*}\psi^{*\prime\prime} + (V(x) - E^*)\psi^*(x) = 0 \tag{38}$$

where E^* stands for the *perturbed* ground state energy, integration over x as previously yields

$$E^* = \int dx\ V(x)\psi^*(x) \tag{39}$$

and thus expression (36) transforms into an identity. Therefore, $\psi^*(x)$ is also the solution of our modified Schrödinger equation (eq. (36)) with an energy E^*.

Thus, we have shown that the sampling procedure tends to a steady-state that is equal (within the statistical errors) to the solution of a modified problem with an effective mass m^*. Since the effective mass is always lower than the real mass m, the resulting wave function penetrates deeper in the classically forbidden regions, and alternatively decreases in the classically allowed regions. As a consequence, the trial function energy estimate E^* (i.e. equ. (39)) is clearly overvalued compared to the exact value E_0. This tendency is in qualitative agreement with what was noticed by several authors (see e.g. [22, 26]). It was shown e.g. in ref. [26] that if a fluctuation increases the fraction of walkers in a region where $V(x) < E_0$, the population size tends to increase, so that the term E_T will moderate this trend and decrease the equilibrium distribution relative to $\psi_0(x)$. The consequence is that the equilibrium distribution $\psi^*(x)$ is too small for low $V(x)$, and too high for high $V(x)$. However, this somewhat qualitative result has never been related to an effective mass of the particle. Here, we have devised a method to understand and quantitatively estimate the bias in the wave function and observables. Note that, for $N = 1$, the effective mass is zero, or alternatively there is no potential, so that the particle undergoes free diffusion.

Note that one may calculate the normalization energy estimate (see eq. (27)) by use of the expression of $E[W]$ derived in Appendix A (see eq. (59)), to find

$$\begin{aligned} E_N &= E_0 - \frac{1}{\Delta t}\log\left[1 - \Delta t \int dx\ \psi^*(x)(V(x) - E_0) + \mathcal{O}(\Delta t^2)\right] \\ &= E_0 + \int dx\ \psi^*(x)(V(x) - E_0) + \mathcal{O}(\Delta t) \end{aligned} \tag{40}$$

similar to equation (39). Thus, the normalization energy estimate will also be biased (with the same bias). Now, in order to estimate this energy bias (due to a finite N), we make use of a simple perturbation calculation (expansion in $1/N$). The derivation of the biased wave function $\psi^*(x)$ is reported in Appendix B. At view of equ. (37) and (38), the Hamiltonian of

the modified problem can be written as $H = H_0 + \Delta H$, where $H_0 = T + V$ is the Hamiltonian of the original problem, and $\Delta H = T/N$. Thus, the energy bias can be written as

$$\Delta E = E^* - E_0 = \langle \psi_0 | \Delta H | \psi_0 \rangle = \langle T \rangle_0 / N \ , \tag{41}$$

where $\langle T \rangle_0$ stands for the expectation value of the kinetic energy in the *unperturbed* ground state. Note that this expression proves quite naturally that the energy bias is always positive, as already mentioned. It has been already noticed in ref. [22, 26] that the MC estimator tends to overestimate the ground state energy, and that the bias scales like $\mathcal{O}(N^{-1})$, but its exact form was not known. Equation (41) is checked in Appendix B for the simple case of an harmonic oscillator. It is shown that the perturbed ground state wave function can be written as

$$\psi^*(x) = \psi_0(x) + \frac{1}{8N} \left[\psi_2(x) - \psi_0(x) \right] \tag{42}$$

where $\psi_2(x)$ stands for the second excited state wave function (normalized with our convention). The resulting estimate for the ground state energy is thus given by

$$E^* = E_0 + \frac{1}{N} \langle T \rangle_0 = \omega \left(\frac{1}{2} + \frac{1}{4N} \right) \tag{43}$$

Our result is general, and applies also for many-dimensional problems as well as problems in discrete space (see Section 4). The only condition is that the time-evolution operator $\exp(-H\Delta t)$ can be divided into a diffusion part $\exp(-T\Delta t)$ and a weight $\exp(-V\Delta t)$. The diffusion operator must be such that $\langle 1 | \exp(-T\Delta t) | x \rangle = 1$ for all x, which amounts to say that the associated matrix must be stochastic. One can also extend our result to the case of a stochatic iteration of a matrix (cfr. [22]) for determining the lowest eigenvalue. In this case, following the notation of Section 1, we can see that the random walk tends to a steady state which is the dominant eigenvector of the modified matrix

$$A^*_{ij} = M_{ij} {w_j}^{1-1/N} \tag{44}$$

differing from exact one by a factor $1/N$.

The major assumptions that we have made to obtain (36), (37), and (41) are (*i*) a very small time-step Δt; and (*ii*) statistical independence between the random walkers. As already explained, the second one is the most drastic (it forgets about the replication process), so that we can not hope the method to yield more than the order of magnitude of the bias. For instance, we can calculate the scaling of this bias with different parameters of the problem (see e.g. Section 4). On the other hand, assumption (*i*) has shown to be not very important for reasonably small choice for Δt. Moreover, it is possible to greatly improve the convergence in Δt by using a symmetric form for the breakup (see [27]):

$$\exp(-H\Delta t) = \exp(-V\Delta t/2) \exp(-T\Delta t) \exp(-V\Delta t/2) + \mathcal{O}(\Delta t^3) \ . \tag{45}$$

With this breakup, extrapolation to small Δt's can be unnecessary, and assumption (*i*) has no consequence. Note also that there is no time-step error at all in the GFMC method since the propagator is exactly simulated.

4 Example in a discrete space : pairing Hamiltonian

The purpose of this Section is to show that the previously described bias can be important and indeed scales as $1/N$. We choose to illustrate this point on the so-called pairing Hamiltonian which describes the residual interaction between nucleons in nuclei. Let us consider a many-body system with the Hamiltonian

$$H = \sum_{k=1}^{\Omega} \epsilon_k (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) - G \sum_{k,k'=1}^{\Omega} a_{k'}^\dagger a_{\bar{k}'}^\dagger a_{\bar{k}} a_k \ . \tag{46}$$

where k and $\bar{k}$ are time-reversed conjugate states (with energies ϵ_k), Ω is the total number of conjugate state pairs, and $G(\geq 0)$ stands for the strength of the pairing force. One is interested in calculating the exact ground state energy E_0 for a system of n pairs of particles by a diffusion Monte Carlo procedure (i.e., the nucleon pair diffusion is simulated stochastically). We define the breakup $H = V + T$, with

$$\begin{aligned} V &= \sum_{k=1}^{\Omega} \epsilon_k (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) - E_{\text{sen}} \\ T &= E_{\text{sen}} - G \sum_{k,k'=1}^{\Omega} a_{k'}^\dagger a_{\bar{k}'}^\dagger a_{\bar{k}} a_k \ , \end{aligned} \tag{47}$$

where $E_{\text{sen}} = n(\Omega - n + 1)G$ corresponds to the (absolute value of) the ground-state energy E_0 in the case where all the single particle levels are degenerate (i.e., $\epsilon_k = 0$ for all k). The operator $\exp(-T\Delta t)$ is then a diffusion operator, as can be seen by checking that $\sum_{C'} \langle C'|T^l|C\rangle = 0$ for all integer $l > 0$ and for any configuration C. The diffusion follows a Poisson law (see [28, 29]), and $\exp(-V\Delta t)$ is used as a weight since it is diagonal in C space. In analogy with equation (31), the ground state energy is given by

$$E_0 = \sum_C V(C)\psi_0(C) \tag{48}$$

where $\psi_0(C)$ is the component of C in the exact ground state, and $V(C) = \langle C|V|C\rangle$. Thus, a MC trial estimator for E_0 is given by

$$E_T = \frac{1}{N} \sum_{i=1}^{N} V(C_i) \ , \tag{49}$$

where the $\{C_i\}$ are the configurations generated by the MC run. In fact, there are two ways to interpret the sum on the right hand side as will be explained in Section 5.1. As shown previously, this estimator is biased because the $\{C_i\}$ ensemble does not distribute as $\psi_0(C)$. Of course, a growth estimator for E_0 can also been used in this case, and it is biased as well. Here, we are essentially interested in the behaviour for different limiting cases (weak or strong

pairing), and in the scaling with Ω. We have trivially $T = 0$ for the limiting case $G = 0$ (i.e., no pairing), so that the bias disappears. For degenerate states (i.e. $\epsilon_k = 0$ for all k), we have $V = E_0 = -E_{\rm sen}$, so that clearly $\langle T \rangle = 0$ and the bias is again zero. Thus, the bias vanishes for both limiting cases, and tends to a maximum somewhere in between as noticed numerically in [29]. Furthermore, when the model space dimension Ω increases, with G varying such that the ground state energy is approximately independent of Ω, it is easy to show that $\langle T \rangle$ is approximately proportional to $E_{\rm sen}$. Thus the energy bias scales as Ω^2/N, which explains that it becomes important for large model spaces (see [29]).

In Figure 1, we give the dependence of the computed ground state energy for a typical model system with $n = 12$ pairs of particles in $\Omega = 24$ equispaced doubly-degenerate levels, with a pairing strength $G = 0.5$ (expressed in units of the level spacing). The data points of interest to us here (i.e., with $k = 0$, as explained in Section 5.4) have been fitted to a linear law in $1/N$; one sees that the fit is very good. To get one percent accuracy without extrapolation, it is necessary to take $N \geq 3000$. The data shown are for the naïve growth estimator, but the other estimators (such as E_T with different ways to calculate the sum) give almost identical results; their agreement does *not* provide a test of the reliability of the method. We have also considered other observables than the energy. In general, their estimators have still larger biases, so that it is necessary to go to larger values of N before being able to extrapolate in $1/N$.

5 Solutions to suppress the bias

Section 3 showed how to estimate the magnitude of the bias both for the wave function and for observables such as the energy. If the bias is comparable to or larger than the statistical error, it is necessary to remove it or at least reduce it. The simplest procedure consists in extrapolating to the $N \to \infty$ limit. Other possibilities include changing the evolution or replication procedure so that the bias on the wave function is of order $1/N^2$ or smaller. We discuss these three choices successively, and illustrate them on simple model Hamiltonians. Finally, we consider modifications of the estimator itself which remove most of the bias whether or not ψ^* is close to ψ_0.

5.1 Extrapolation in N

We saw in Section 4 that an energy estimator extrapolates well with a $1/N$ scaling for large N. For a different observable or a different problem, the onset of the $1/N$ scaling will occur at smaller or larger values of N. In this Section, we quantify the convergence of ψ^* to ψ_0 as $N \to \infty$. To do this, we measure how various moments of the distribution ψ^* converge to their $N = \infty$ limit. We have considered the observables

$$\mu_k \equiv \int_{-\infty}^{\infty} x^k \psi^*(x) dx \simeq \frac{\sum_i w(x_i) x_i'^k}{\sum_i w(x_i)} \tag{50}$$

for a one-dimensional anharmonic oscillator to check the convergence. The potential was taken to be $V(x) = x^4 - x^2 + x/2$, with $\hbar = m = 1$. As already mentioned, there are two possible ways to interpret this ratio. In the Kalos prescription [23], the ratio is taken at each time step, and then averaged over iterations. In the Ceperley-Kalos prescription [18, 19], the numerator and denominator are averaged separately before taking ratios, with the expectation that this will reduce the bias. However, we find that the bias is nearly identical for the two prescriptions. It is present in the wave function ψ^*, and not just in observables, with a convergence which is linear in $1/N$, as predicted by the theory. Figure 2 shows the convergence of the first four moments for the Ceperley-Kalos prescription using the standard replication [17]. Nearly identical results are obtained with the Kalos prescription. Because this model is so simple, it is possible to use the $1/N$ extrapolation from very small values of N. However, for non-toy problems such as the one described in Section 4, much larger values of N are necessary.

Doing an extrapolation in N is inconvenient for two reasons. First, it is necessary to check that the values of N considered are in the $1/N$ scaling regime. Thus at least three values of N have to be used. Second, the extrapolation magnifies the statistical errors. For instance, if the data points at N and $2N$ are used in the linear extrapolation, and if each data point has a statistical error of σ, the extrapolated value has a statistical error of $\sqrt{5}\sigma$. If it were possible to eliminate the bias, the computer time could be used entirely for the data point at N, leading to a statistical error of $\sigma/\sqrt{2}$. The ratio of the statistical errors in the two cases is then equal to $\sqrt{10}$, which corresponds to a factor of 10 of computer time. This provides strong motivation for searching for bias-free methods.

5.2 Modifying the evolution operator

It is well known that if the evolution is done using a guided random walk (also sometimes called importance sampling, or generalized Feynman-Kac), the convergence of ψ^* towards ψ_0 can be improved. In fact, if the guiding (cf. Section 2) is done using ψ_0, the weights have no variance, so that no replication is needed, and one obtains $\psi^* = \psi_0$. Of course, in practice ψ_0 is not known, so a natural question is whether this is the only choice of guiding which leads to ψ_0, particularly in the presence of replication. Since it is difficult to analyze the effects induced by almost all replication procedures, we consider here the less ambitious goal of finding an evolution/replication procedure for which ψ^* converges towards ψ_0 faster than $1/N$.

Our approach is empirical, numerical, but motivated by the perturbative calculations of Section 3. There we saw that, for a particular choice of replication, ψ^* was the solution of a Schrödinger equation with a perturbed mass. This suggests that by using a different value of the mass in the evolution operator, it may be possible to eliminate the $1/N$ bias. Unfortunately, as previously remarked, the replication used in the theoretical analysis is not readily implemented in practice. For other replications, the analysis is not feasible because the random walkers become correlated, so that the effective ensemble size N_{eff} is less than the number of walkers. (For instance, we will see in Section 5.3 that in the $\Delta t \to 0$ limit, the Hetherington replication procedure [22] leads to $N_{\text{eff}} = 1$, i.e., the configurations at a given time are different only by

order Δt.) Nevertheless, the analytic calculations are suggestive, so we consider rescaling the time step appearing in the diffusion operator using

$$\Delta t \to \Delta t(1 - 1/N_{\text{eff}}) \ . \tag{51}$$

Here, N_{eff} is something like the number of independent configurations, but in practice it is a free parameter which we set so that the first moment has no bias. Then we determine numerically the convergence of the other moments of ψ^* (cf. the study in Section 5.1) to their $N \to \infty$ limit. Though we did find that the correction improved the results, they were erratic in the sense that there was no unique value of N_{eff} which gave the correct value for all the moments. In particular the scaling of the biases remained proportional to $1/N$. We checked this within the two interpretations of observables (taking average of ratios or ratios of averages), and using the standard replication. No doubt the failure to find a $1/N^2$ convergence arises because the theoretical calculations supposed a different replication, and because the correction must depend on the form of the replication. A different kind of replication was studied by Hetherington [22]; he estimated the form of the bias neglecting correlations within walkers. His analysis suggests that the $1/N$ term of the bias can be removed by the modification (cf. the matrix notation in Section 1)

$$w_i \to w_i(1 - w_i/N_{\text{eff}}) \ . \tag{52}$$

We have numerically investigated this possibility, with the same negative result as above for the standard replication. In summary, we have not been able to find a simple prescription for removing the leading term of the bias, but think it is worth persuing.

5.3 Modifying the replication procedure

Above we considered possible modifications of the evolution operator to remove the $1/N$ bias in ψ^*. The bias is also affected by the replication procedure. Since there is no analytic work here to guide us, we will simply determine the magnitude of the bias for three often used replication methods: that of Hetherington [22], the "standard" method [9, 17, 18, 23], and an "improved" method due to Nightinghale and Blöte [20]. For completeness, we first describe these three methods, and then summarize in Figure 3 their influences on the bias.

In the Hetherington approach, the N weights of the configurations after evolution by Δt are rescaled to give a probability distribution; then N new configurations are chosen at random from this probability distribution and each is given weight 1. Although it is rarely used, this method has the advantage of keeping N fixed, and this enabled Hetherington to estimate the scaling of the bias (neglecting correlation effects). The main disadvantage is that as $\Delta t \to 0$, the replication is no longer effective: in fact, it is no longer affected by the potential, the diffusion occurs as in the absence of potential, and all the configurations become identical to within Δt. The effective number of random walkers is then equal to 1 and there is no guiding at all. With this replication, N must scale as $1/\Delta t$ to keep the bias constant as $\Delta t \to 0$.

The standard replication procedure is best presented in a continuous time formalism [17]. Starting with equation (15), we see that the potential term gives a probability per unit time to

either die or to be born. Thus for each time step Δt, $(V(x)-E_0)\Delta t$ gives the decrease/increase in the population at that point in x and for that time interval. If it is negative, a new configuration is to be created at that x with that probability; if it is positive, the configuration has a death probability. In practice, this birth and death process is implemented [23] by picking a random number ξ between 0 and 1 and duplicating (or killing) whenever $\xi < |(V(x) - E_0)\Delta t|$.

We can now motivate the improved replication of Nightinghale and Blöte [20]. Imagine using the above standard method and calculating the growth estimator from

$$e^{-\Delta t E_0} \simeq \left\langle \frac{\sum_{i=1}^{N(n)} w_i}{N(n)} \right\rangle_{\text{before}} = \left\langle \frac{N(n+1)}{N(n)} \right\rangle_{\text{after}} \tag{53}$$

where $N(n)$ is the number of configurations at time step n, and the average is over time steps. The first estimator is evaluated after evolution but before replication. After replication, one obtains a second estimator because $\sum_{i=1}^{N(n)} w_i$ is replaced by $N(n+1)$ which is simply a random variable whose average is $\sum_{i=1}^{N(n)} w_i$. We see therefore that measuring observables after the replication introduces unnecessary noise. Nightinghale and Blöte realized that it was possible to introduce a replication which introduced no noise at all into the total population weight so that the growth estimator is the same before and after replication. The idea is to keep weighted configurations, and to do the birth/death processes only when the weights have varied significantly. Their replication is defined as follows. First, for a birth process, one duplicates a configuration and reduces its weight by a factor 2. (Note that this is deterministic rather than stochastic.) Second, for a death process, given two configurations of weight w_i and w_j, one selects one of them with a probability given by its weight relative to $w_i + w_j$. The other one is killed, while the first is maintained and given the new weight $w_i + w_j$. This procedure preserves exactly the total weight of the population during replication.

How do these replications influence the bias in ψ^* ? Not surprisingly, the three methods lead to biases which scale with $1/N$, but with different coefficients. The Hetherington method gives rise to a bias which scales as $1/(N\Delta t)$, as discussed above, whereas the two other methods have finite $\Delta t \to 0$ limits. In Figure 3, we show the dependence on $1/N$ of the energy of an anharmonic oscillator problem. The different replications all lead to a linear dependence at large N. Note also that there is no improvement in this case when going from the standard to the Nightinghale-Blöte replication. Probably the main advantage of the Nightinghale-Blöte replication is that it is a well defined process; on the contrary, the standard replication can with a low probability lead to an empty population, so its large time behavior leads to incorrect results.

5.4 Modifying the estimator

Once it is realized that ψ^* is inevitably different from ψ_0, it is natural to modify the estimators so as to remove the bias. The idea is to use matrix elements between ψ^* and any given trial wave function ψ_T, while inserting projection operators so that only the ground state components

contribute. For instance, the ratio of matrix elements

$$\frac{\langle\psi_T|e^{-(k+1)\Delta tH}|\psi^*\rangle}{\langle\psi_T|e^{-k\Delta tH}|\psi^*\rangle} = e^{-\Delta tE_0}\left(1+\mathcal{O}(e^{-k\Delta t(E_1-E_0)})\right) \tag{54}$$

leads to a growth estimator of the ground state energy which is unbiased in the $k \to \infty$ limit. The numerator and denominator can be estimated simultaneously (up to the same multiplicative constant) within one MC run. For instance if we assume the weights to be 1 (as in two of the three replications discussed above), the denominator can be estimated using

$$\langle\psi_T|e^{-k\Delta tH}|\psi^*\rangle \simeq \sum_n \sum_{i=1}^{N(n+k)} \psi_T\left(x_i(n+k)\right)\Pi_k(n)\ , \tag{55}$$

where n is the time-step number. In this expression, $\Pi_k(n) = \Pi_{l=n}^{l=n+k-1}\pi(l)$, and $\pi(l)$ is the factor by which the weights are rescaled before replication number l. This factor is used to maintain the population size around some average value. Whenever estimators are derived from ratios of matrix elements as we have done here, it is clear that the correct procedure is to average first and take ratios second, rather than take ratios first. This is a way of justifying the Ceperley-Kalos [19] improvement of the way Kalos [23] calculated the energy. Nightinghale and Blöte [20] introduced the same estimators, which they motivated by "undoing" the normalization used in the replications. It seems to us that the best way to understand both why the method works and its limitations is to realize that one is estimating matrix elements.

Given the above estimator as a function of k, the exact answer (up to statistical errors) is obtained by extracting the $k \to \infty$ limit, with an exponential convergence. However, it is important to note that in this limit, the estimators for both the numerator and the denominator grow exponentially, so one must in practice extract the limiting behavior from small values of k. In Figure 1, we show the results using these modified estimators for the pairing Hamiltonian problem (cf. Section 4). To compare the usefulness of the method for a realistic problem, we have used the same statistics for the points with $k = 0$ (i.e., the estimator used in Section 4), and for the other values of k. We see that when the error in the naïve method is large (too small N), the above estimator greatly improves things. However, when the bias is already small with the $k = 0$ estimator, increasing k rapildy reaches noise levels where there is no improvement.

A consequence of this is that it is possible to introduce unbiased (up to exponentially small corrections) estimators for local operators which do not commute with the Hamiltonian. Let O be a general (local) observable; in the standard method, an estimator for its expectation value is obtained from

$$\langle\psi_0|O|\psi_0\rangle \simeq \frac{<\psi_T|e^{-\tau H}O|\psi_0>}{<\psi_T|e^{-\tau H}|\psi_0>}\ , \tag{56}$$

where τ should be taken large enough to eliminate contributions from excited states. Since we know that in fact $\psi^* \neq \psi_0$, a computable observable is

$$\frac{<\psi_T|e^{-\tau H}Oe^{-k\Delta tH}|\psi^*>}{<\psi_T|e^{-(\tau+k\Delta t)H}|\psi^*>}\ . \tag{57}$$

Then the bias in the numerical estimator is due to extrapolating to the $\tau, k \to \infty$ limit, and to the fact that with finite statistics, the numerator and denominator are correlated; this last contribution can be made arbitrarily small by extending the length of the run.

6 Conclusion

We have shown that projection MC methods for calculating ground state properties are affected by a bias related to the finite size of the population of random walkers. The source of this bias is the replication which is introduced to avoid an exponential growth/decay of the population size. This difficulty occurs whenever the propagator differs from a diffusion operator (i.e., $\sum_i A_{ij}$ varies with j in matrix notation). The propagation of the population of walkers then converges to a steady-state distribution which we call ψ^*, and which is not equal to the exact ground state ψ_0. Our analytic calculation shows that, for a particular replication procedure, ψ^* corresponds to the ground state of a modified Schrödinger equation in which the mass m is replaced by an effective mass $m^* = m(1 - 1/N)$ for a population of walkers of size N. As a consequence, the bias on any observable scales as $1/N$. Nevertheless, for the replications used in practice, we have not been able to obtain the detailed form of the correction, so this is still an open problem. Finally, we have considered different strategies to eliminate the bias, namely extrapolation in N, modifications of the evolution/replication procedure, or the introduction of new observables. This latter approach proves to be the most efficient as it can deal with any $\psi^* \neq \psi_0$.

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Appendices

A Derivation of the moments of W, F, and F_N

Let us present the calculation of the various moments of W, F, and F_N. (The calculation requires only keeping terms of first-order terms in Δt in the expansion of $w(x)$ and $P(x', x)$.) In order to calculate the expectation value of F_N, we expand in powers of Δt the expression for F_N, leading to

$$E[F_N] = \frac{E[F]}{E[W]}\left[1 - \frac{\mathrm{Cov}[F, W]}{E[F]\ E[W]} + \frac{\mathrm{Var}[W]}{E[W]^2}\right] + \mathcal{O}(\Delta t^2)\ , \tag{58}$$

where Cov[] and Var[] stand for the covariance and the variance of the arguments, respectively. We are interested first in calculating the expectation value of both estimators W and F. We have for the expectation value of W

$$E[W] = E[w(x)] = e^{-\Delta t\ E_0}\left[1 - \Delta t \int dx\ \psi(x)(V(x) - E_0) + \mathcal{O}(\Delta t^2)\right] \tag{59}$$

where we have made use of the normalization of $P(x', x)$, and we have only kept the contribution of first-order terms in Δt in the expansion of $w(x)$. Note that the expectation value is calculated by use of

$$E[X] = \int\int dx\ dx'\ P(x', x)\psi(x)X(x, x') \tag{60}$$

For the expectation value of $F(\tilde{x})$, we have

$$\begin{aligned} E[F(\tilde{x})] &= E[w(x)\delta(\tilde{x} - x')] \\ &= \psi(\tilde{x})w(\tilde{x}) + \frac{\Delta t}{2m}\left[\psi(x)w(x)\right]''_{x=\tilde{x}} \\ &= e^{-\Delta t\ E_0}\left[\psi(\tilde{x}) + \frac{\Delta t}{2m}\psi''(\tilde{x}) - \Delta t\ (V(\tilde{x}) - E_0)\psi(\tilde{x}) + \mathcal{O}(\Delta t^2)\right] \end{aligned} \tag{61}$$

where we have kept the second-order term in the gaussian random walk expansion, yielding a term in Δt. Note that all the derivatives of $w(x)$ are neglected because they give one supplementary order in Δt. The ratio of the expectation values of both estimators then expresses as

$$\begin{aligned} \frac{E[F(\tilde{x})]}{E[W]} = \psi(\tilde{x}) + \frac{\Delta t}{2m}\psi''(\tilde{x}) - \Delta t\ (V(\tilde{x}) - E_0)\psi(\tilde{x}) \\ + \Delta t\ \psi(\tilde{x}) \int dx\ \psi(x)(V(x) - E_0) + \mathcal{O}(\Delta t^2) \end{aligned} \tag{62}$$

when neglecting second- (and higher-) order terms in Δt. Assuming that the points x_i are independent, we get for the covariance of F and W

$$\begin{aligned}\mathrm{Cov}[F(\tilde{x}), W] &= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\mathrm{Cov}[w(x_i)\delta(\tilde{x}-x_i'), w(x_j)] \\ &= \frac{1}{N}\left[E[w^2(x)\delta(\tilde{x}-x')] - E[F(\tilde{x})]\ E[W]\right] \qquad (63)\end{aligned}$$

It is worth noticing that this independence assumption is a crucial point of the calculation, as explained in Section 3.1. Now, we have thus to calculate

$$\begin{aligned}E[w^2(x)\delta(\tilde{x}-x')] &= \psi(\tilde{x})w^2(\tilde{x}) + \frac{\Delta t}{2m}\left[\psi(x)w^2(x)\right]''_{x=\tilde{x}} \\ &= e^{-2\Delta t\ E_0}\left[\psi(\tilde{x}) + \frac{\Delta t}{2m}\psi''(\tilde{x}) - 2\Delta t\ (V(\tilde{x})-E_0)\psi(\tilde{x}) + \mathcal{O}(\Delta t^2)\right] \qquad (64)\end{aligned}$$

Finally, we can express the covariance of F and W as

$$\begin{aligned}&\mathrm{Cov}[F(\tilde{x}), W] = \\ &-\frac{1}{N}e^{-2\Delta t\ E_0}\left[\Delta t\ (V(\tilde{x})-E_0)\psi(\tilde{x}) - \Delta t\ \psi(\tilde{x})\int dx\ (V(x)-E_0)\psi(x) + \mathcal{O}(\Delta t^2)\right] \qquad (65)\end{aligned}$$

Now, assuming the x_i to be independent as previously, we have for the variance of W

$$\mathrm{Var}[W] = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\mathrm{Cov}[w(x_i), w(x_j)] = \frac{1}{N}\left[E[w^2(x)] - E[W]^2\right] \qquad (66)$$

Using

$$E[w^2(x)] = e^{-2\Delta t\ E_0}\left[1 - 2\Delta t\ \int dx\ \psi(x)(V(x)-E_0) + \mathcal{O}(\Delta t^2)\right] \qquad (67)$$

we get

$$\mathrm{Var}[W] = \frac{1}{N}e^{-2\Delta t\ E_0}\ \mathcal{O}(\Delta t^2) \qquad (68)$$

Thus the contribution of the third term in the right-hand side of equ. (58) is of the order Δt^2, and can be neglected. Finally, using (58), (59), (61), (62), and (65), we obtain for the expectation value of F_N,

$$\begin{aligned}E[F_N(\tilde{x})] = \psi(\tilde{x}) &+ \frac{\Delta t}{2m}\psi''(\tilde{x}) - \Delta t\ (V(\tilde{x})-E_0)\psi(\tilde{x}) + \Delta t\ \psi(\tilde{x})\int dx\ \psi(x)(V(x)-E_0) \\ &+\frac{\Delta t}{N}(V(\tilde{x})-E_0)\psi(\tilde{x}) - \frac{\Delta t}{N}\psi(\tilde{x})\int dx\ \psi(x)(V(x)-E_0) + \mathcal{O}(\Delta t^2) \qquad (69)\end{aligned}$$

B Bias in the wave function

We are now searching for an expression of the biased wave function $\psi^*(x)$. Using equ. (39), the energy bias is written as

$$\Delta E = E^* - E_0 = \int dx\ V(x)\ (\psi^*(x) - \psi_0(x)) \tag{70}$$

Let us write

$$\psi^*(x) = \psi_0(x) + \frac{1}{N} f(x) \tag{71}$$

since it is clear that the sampling introduces a perturbation of the order $1/N$ (via the effective mass) on the wave function $\psi^*(x)$. Note that the normalization of $\psi^*(x)$ imposes the condition

$$\int f(x)\ dx = 0 \tag{72}$$

As a consequence of (70), it is evident that the energy bias will also be of the order $1/N$, but we are interested here in an absolute value (not only the scaling with N). By inserting (71) into eq. (36), and keeping only the first-order term in the expansion in $1/N$, one obtains the equation for $f(x)$

$$-\frac{1}{2m} f'' + (V(x) - E_0) f(x) - (V(x) - E_0)\psi_0(x) - \psi_0(x) \int dx\ V(x)\ f(x) = 0 \tag{73}$$

where we have made use of eq. (23) and (31). It is apparent from eq. (70) that the forth term can be written $\psi_0(x)\ N\ \Delta E$, and thus this equation can also be used in order to deduce ΔE. Let us expand the perturbation component $f(x)$ in a series of the eigenfunctions of the *unperturbed* Schrödinger equation,

$$f(x) = \sum_{n=0}^{\infty} a_n\ \psi_n(x) \qquad \text{with } -\frac{1}{2m}\psi_n'' + (V(x) - E_n)\psi_n(x) = 0 \tag{74}$$

Note that the eigenfunctions $\psi_n(x)$ have an arbitrary normalization here, that is $\int \psi_n(x)\ dx = I_n$, so that equation (72) imposes that

$$\sum_{n=0}^{\infty} a_n I_n = 0 \tag{75}$$

Insertion in eq. (73) yields

$$\sum_{n=0}^{\infty} a_n (E_n - E_0)\psi_n(x) = [V(x) - E_0 + N\ \Delta E]\ \psi_0(x) \tag{76}$$

which must be valid for all x. Thus, in order to determine the coefficients a_n, the right-hand side of eq. (76) has to be expanded in a series of the $\psi_n(x)$. First, we can calculate the energy bias ΔE by writing the equation corresponding to $n = 0$:

$$\int |\psi_0(x)|^2\ [V(x) - E_0 + N\ \Delta E]\ dx = 0 \tag{77}$$

Thus we have

$$\Delta E = \frac{1}{N}\left[E_0 - \langle V\rangle_0\right] = \frac{\langle T\rangle_0}{N} \tag{78}$$

where

$$\langle V\rangle_0 = \frac{\int |\psi_0(x)|^2\, V(x)\, dx}{\int |\psi_0(x)|^2\, dx} \tag{79}$$

stands for the expectation value of the potential energy in the unperturbed ground state, while $\langle T\rangle_0$ is the similar expression for the kinetic energy. Note that this expression is of course equivalent to equation (41). The other terms ($n \neq 0$) of the expansion along with the obtained value for ΔE can be used in order to evaluate the a_n's. Then a_0 is obtained using (75), and thus we can precisely determine $f(x)$.

Let us check our results in the simple case of an harmonic oscillator, with a potential

$$V(x) = \frac{1}{2}m\omega^2 x^2 \tag{80}$$

The normalized (with our convention) ground state wave function is given by

$$\psi_0(x) = \sqrt{\frac{\alpha^2}{2\pi}}\, e^{-\frac{\alpha^2 x^2}{2}} \qquad \text{with } \alpha^2 \equiv \frac{m\omega}{\hbar} \tag{81}$$

Our estimate for the ground state energy is then

$$E_0 = \int V(x)\psi_0(x)\, dx = \frac{\hbar\omega}{2} \tag{82}$$

It can be checked that the perturbation component of the wave function can be simply written in this case as

$$f(x) = a_0\psi_0(x) + a_2\psi_2(x) \tag{83}$$

where $\psi_2(x)$ is the normalized wave function of the second excited state, that is

$$\psi_2(x) = \sqrt{\frac{\alpha^2}{2\pi}}\,(2\alpha^2 x^2 - 1)e^{-\frac{\alpha^2 x^2}{2}} \tag{84}$$

with an energy

$$E_2 = \int V(x)\psi_2(x)\, dx = \frac{5\hbar\omega}{2} \tag{85}$$

Then, equations (72) and (73) are verified on the condition that $a_2 = -a_0 = 1/8$, so that $f(x)$ is exactly given by

$$f(x) = \frac{1}{4}\sqrt{\frac{\alpha^2}{2\pi}}\,(\alpha^2 x^2 - 1)e^{-\frac{\alpha^2 x^2}{2}} \tag{86}$$

Finally, the estimate for the energy bias can be calculated as

$$\Delta E = \frac{1}{N}\int dx\; V(x)(a_0\psi_0(x) + a_2\psi_2(x)) = \frac{1}{N}\left[\frac{E_2 - E_0}{8}\right] = \frac{1}{N}\left[\frac{\hbar\omega}{4}\right] \tag{87}$$

Now, using virial theorem for the harmonic oscillator $\langle V\rangle = \langle T\rangle = E_0/2$, and replacing into equation (78), one finds the same expression for the bias.

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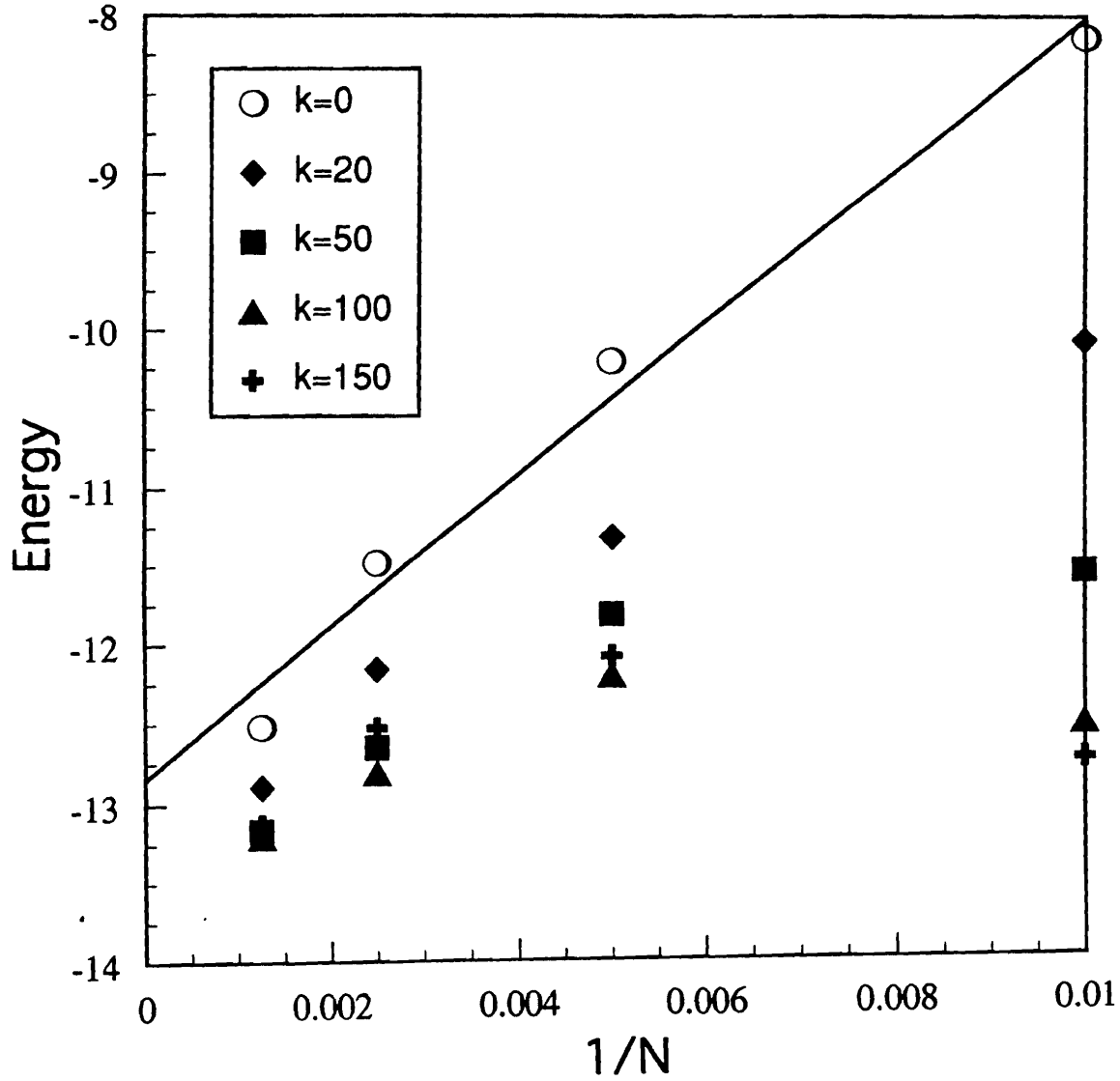
Figure captions

Figure 1: Growth estimator for the ground state energy as a function of $1/N$, with N being the size of the population of random walkers. The data fit to a line corresponds to the simple estimator (i.e., $k = 0$). The corrected estimators (following [20], as discussed in 5.4) for $k = 20, 50, 100, 150$ are also shown. The model consists in $n = 12$ pairs of particles placed in $\Omega = 24$ equispaced doubly-degenerate levels, and interacting through a pairing force of strength $G = 0.5$ (see [28, 29]). The exact value of the energy is 13.096 (expressed in units of the level spacing).

Figure 2: Four first reduced moments ($\mu_k/\mu_k^{\text{exact}}$, with $k = 1, \cdots 4$) as a function of $1/N$, with N being the size of the population of random walkers. The system is an 1-D anharmonic potential $V(x) = x^4 - x^2 + x/2$. (The used time-step is $\Delta t = 0.05$).

Figure 3: Estimator of the energy as a function of $1/N$, for the three different types of replication procedures (with the same time step $\Delta t = 0.05$). Std.: standard method; N-B: Nightinghale-Blote; H-I: Hetherington. The Δt-dependence of the Hetherington replication is also illustrated by the dashed line at $\Delta t = 0.025$ (H-II). The system is an 1-D anharmonic potential $V(x) = x^4 - x^2 + x/2$.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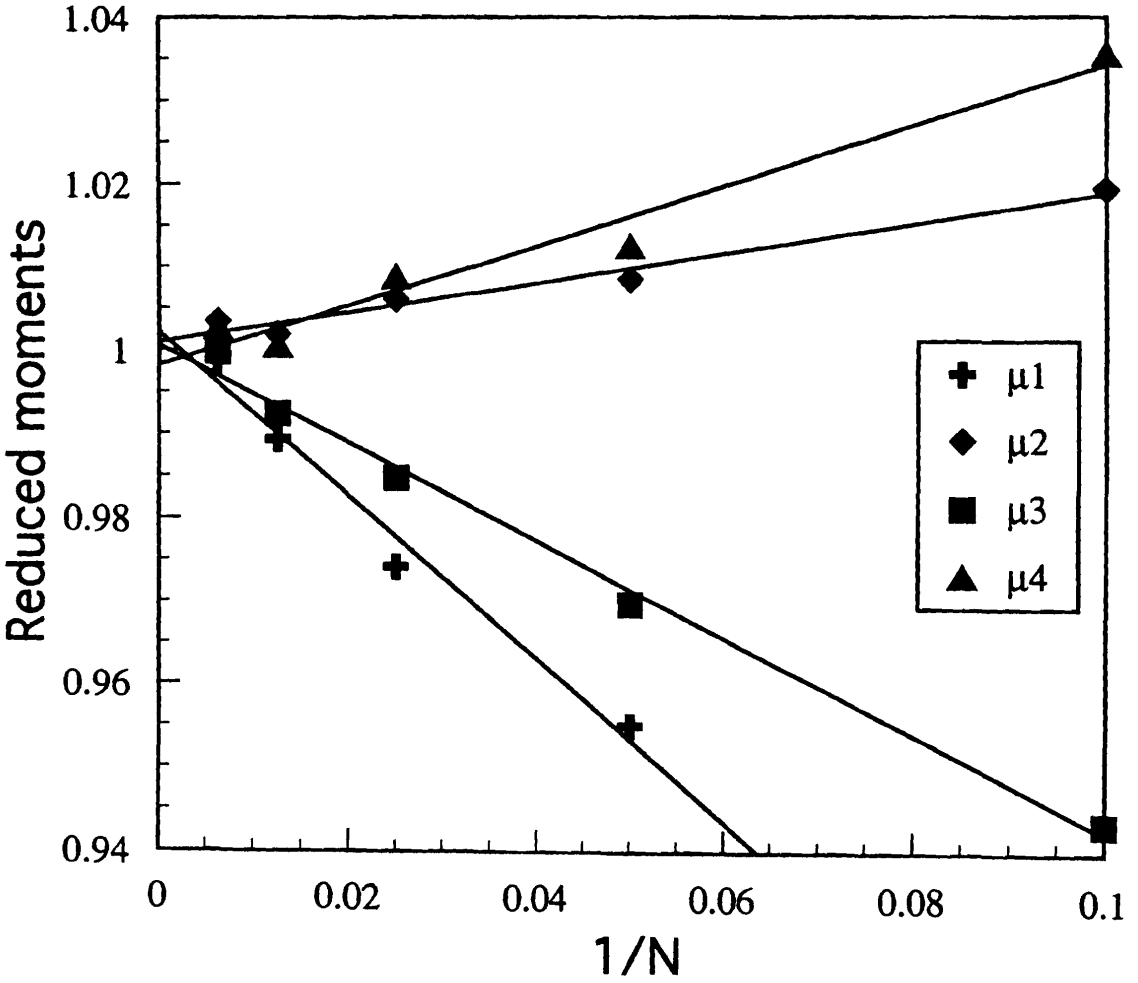
k=20
k=50
k=100
k=150
Energy
1/N
-8
-9
-10
-11
-12
-13
-14
0
0.002
0.004
0.006
0.008
0.01

N. Sep E

Fig. 1



N. Cerf
O. Martin

Fig 2

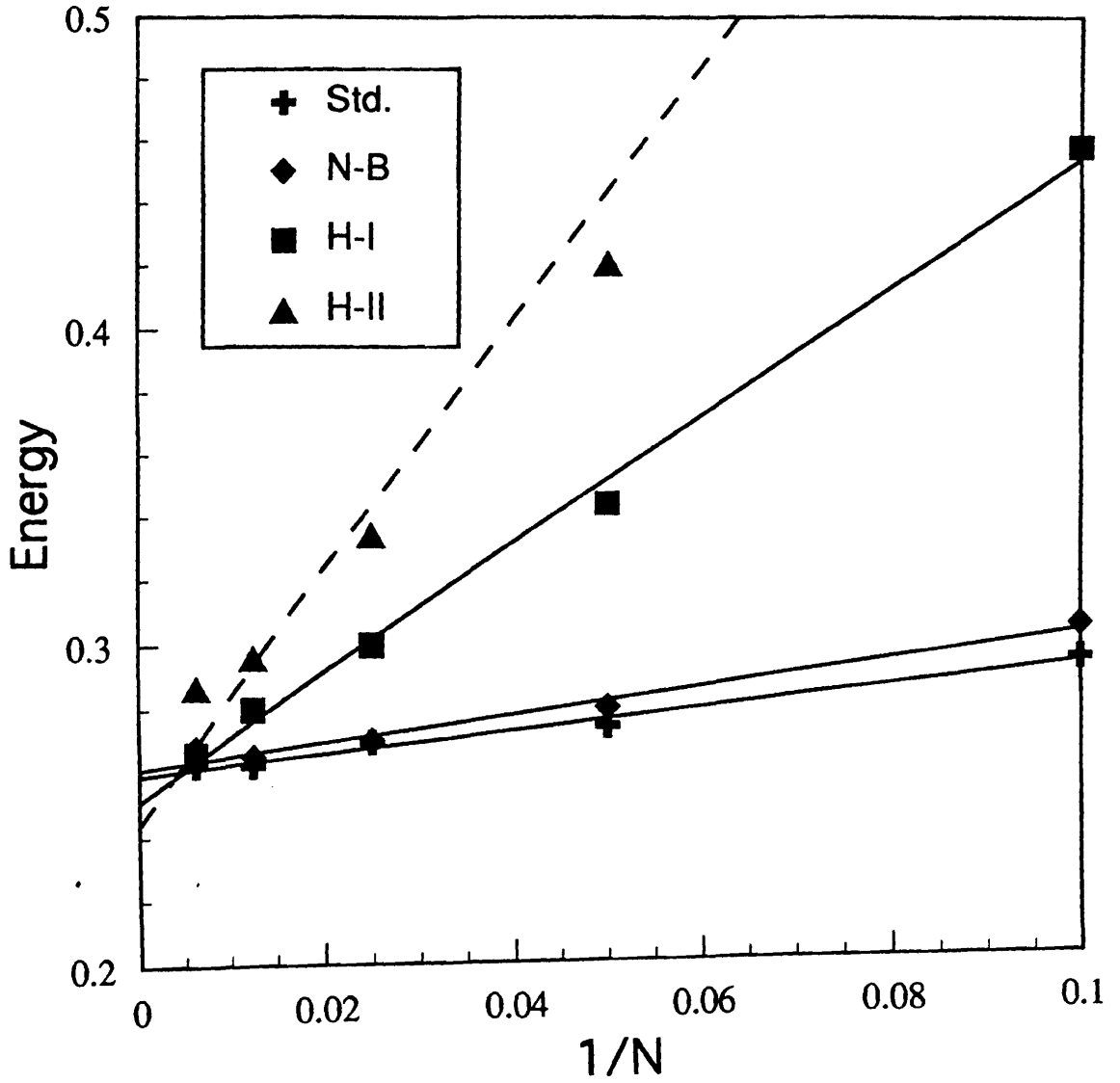


Fig 3

Al. cerf