*Fluctuating Paths and Fields*, Eds. W. Janke, A. Pelster, H.-J. Schmidt, and M. Bachmann (World Scientific, Singapore, 2001).

# THE FEYNMAN PATH GOES MONTE CARLO

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Path-integral Monte Carlo (PIMC) simulations have become an important tool for the investigation of the statistical mechanics of quantum systems. I discuss some of the history of applying the Monte Carlo method to non-relativistic quantum systems in path-integral representation. The principle feasibility of the method was well established by the early eighties, a number of algorithmic improvements have been introduced in the last two decades.

## 1 Introduction

Feynman's classic paper of 1948 presented a *Space-Time Approach to Non-Relativistic Quantum Mechanics* [1], or, in Hagen Kleinert's words [2], "an all-time global approach to the calculation of quantum mechanical amplitudes". Within the philosophy of this approach, we must find, as Kleinert often stressed, "all properties, including the Schrödinger wave functions, from the globally determined time displacement amplitude". The Feynman path, governed by the classical Lagrangian of the quantum system, is the very object we need to study if we want to establish a truly independent alternative to Schrödinger's equation. In avoiding the operator formalism, the sum over paths provides an independent conceptual link between quantum and classical mechanics.

Another attractive feature of the path-integral formulation of quantum mechanics is that it allows to establish a bridge between quantum mechanics and statistical mechanics. Technically, the oscillating exponential of the time-displacement amplitude turns into a positive Boltzmann weight if the paths

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are expressed in imaginary time. The quantum mechanical propagator thus turns into the quantum statistical density matrix. It is this very feature which allows the application of methods of classical statistical mechanics, notably the Monte Carlo method, to quantum systems.

The Monte Carlo method came into being roughly around the same time as the Feynman path. Anecdotally, the idea of gaining insight into a complex phenomenon by making various trials and studying the proportions of the respective outcomes occurred to Stanislaw Ulam while playing solitaire during an illness in 1946 [3]. The immediate application was, of course, the problem of neutron diffusion studied in Los Alamos at that time. The name of the procedure first appeared in print in a classic paper by Metropolis and Ulam in 1949 [4], where the authors explicitly mentioned that the method they presented as a statistical approach to the study of integro-differential equations would sometimes be referred to as the Monte Carlo method. In classical statistical mechanics it quickly became a standard calculation tool.

## 2 Where's Monte Carlo?

The object of interest in Monte Carlo evaluations of Feynman's path integral is the quantum statistical partition function $\mathcal{Z}$ given, in operator language, by the trace of the density operator $\exp(-\beta\hat{H})$ of the canonical ensemble ($\beta = 1/k_{\mathrm{B}}T$) associated with a Hamilton operator describing $N$ particles of mass $m_i$ moving under the influence of a potential $V$:

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{\vec{p}}_i^{\,2}}{2m_i} + V(\hat{\vec{r}}_1, \ldots, \hat{\vec{r}}_N). \tag{1}$$

Expressed as a Feynman integral, the density matrix elements read

$$\langle \mathbf{r}| \exp(-\beta\hat{H})|\mathbf{r}'\rangle = \int_{\mathbf{r}(0)=\mathbf{r}}^{\mathbf{r}(\hbar\beta)=\mathbf{r}'} \mathcal{D}\mathbf{r}(\tau) \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} L\left( \{\dot{\vec{r}}_i(\tau), \vec{r}_i(\tau)\} \right) d\tau \right\}, \tag{2}$$

where $\mathbf{r} \equiv \{\vec{r}_1, \ldots, \vec{r}_N\}$ and $L$ denotes the classical Lagrangian

$$L\left( \{\dot{\vec{r}}_i(\tau), \vec{r}_i(\tau)\} \right) = \sum_{i=1}^{N} \frac{m_i}{2} \dot{r}_i^2 + V(\vec{r}_1, \ldots, \vec{r}_N(\tau)) \tag{3}$$

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expressed in imaginary time $\tau$.[a] The particles are assumed to be distinguishable. To evaluate the trace, we only need to set $\mathbf{r} = \mathbf{r}'$ and integrate over $\mathbf{r}$. To take into account Bose or Fermi statistics for indistinguishable particles, the partition function splits into a sum of the direct Boltzmann part and parts with permuted endpoints.

The right hand side of Eq. (2) is a path integral for the $3N$ functions $\mathbf{r}$. The idea of a Monte Carlo evaluation of this quantity is to sample these paths stochastically and to get (approximate) information about the quantum statistics of the system by averaging over the finite set of paths generated in the sampling process.

Monte Carlo data always come with error bars and, in general, the errors associated with numerical Monte Carlo data stem from two distinct sources. A *systematic* error of Monte Carlo evaluations of the path integral follows from the need to identify the paths by a finite amount of computer information. This can be done by discretizing the paths at some set of points in the interval $(0, \hbar\beta)$. For a single particle moving in one dimension, the simplest discrete time approximation for $L$ time slices reads ($\epsilon = \hbar\beta/L$)

$$\langle x|\exp(-\beta\hat{H})|x'\rangle = \lim_{L\to\infty} \frac{1}{A}\prod_{j=1}^{L-1}\left[\int \frac{dx_j}{A}\right] \exp\left\{-\frac{1}{\hbar}\sum_{j=1}^{L}\left[\frac{m}{2}\frac{(x_j - x_{j-1})^2}{\epsilon} + \epsilon V(x_{j-1})\right]\right\}, \quad (4)$$

where $A = (2\pi\hbar\epsilon/m)^{1/2}$, $x_0 = x$ and $x_L = x'$. Alternatively, one may expand the individual paths in terms of an orthogonal function basis, e.g. by the Fourier decomposition

$$x(\tau) = x + \frac{(x' - x)\tau}{\hbar\beta} + \sum_{k=1}^{\infty} a_k \sin\frac{k\pi\tau}{\hbar\beta}, \quad (5)$$

and express the density matrix as

$$\langle x|\exp(-\beta\hat{H})|x'\rangle = \lim_{L'\to\infty} J \exp\left\{-\frac{m}{2\hbar^2\beta}(x - x')^2\right\}$$

[a]There have been attempts to apply the Monte Carlo method to path integrals also for real time. However, due to the oscillating exponential one then has to deal with problems of numerical cancellation, and it is much harder to obtain results of some numerical accuracy. Therefore, I shall here restrict myself to Monte Carlo working in imaginary time.

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$$\times \int \prod_{k=1}^{L'} da_k \exp\left\{-\frac{a_k^2}{2\sigma_k^2}\right\} \times \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} V(x(\tau))d\tau\right\}, \tag{6}$$

where $\sigma_k = [2\hbar^2\beta/m(\pi k)^2]^{1/2}$ and $J$ is the Jacobian of the transformation from the integral over all paths to the integral over all Fourier coefficients. A systematic error then arises from the loss of information by the finite number $L$ of points $x_i$ on the discretized time axis or by the finite number $L'$ of Fourier components $a_k$ that are taken into account in the Monte Carlo sampling of the paths.

The other error source of Monte Carlo data is the *statistical* error due to the finite number $N_m$ of paths that form the sample used for evaluating the statistical averages. To make matters worse, the probability of configurations is, in general highly peaked, making an independent sampling of paths highly inefficient in most cases. The remedy is to introduce some way of "importance sampling" where configurations are generated according to their probability given by the exponential in Eq. (2). Statistical averages may then be computed as simple arithmetic means. A way to achieve this is by constructing Markov chains where transition probabilities between configurations are constructed that allow to generate a new configuration from a given one such that in the limit of infinitely many configurations the correct probability distribution of paths results. A very simple and universally applicable algorithm to set up such a Markov chain is the Metropolis algorithm introduced in 1953 [5]. Here a new configuration is obtained by looking at some configuration with only one variable changed and accepting or rejecting it for the sample on the basis of a simple rule that only depends on the respective energies of the two configurations. The advantages of importance sampling on the basis of Markov chains are obtained on the cost that, in general, successive configurations are not statistically independent but autocorrelated. The crucial quantity is the integrated autocorrelation time $\tau_{\mathcal{O}}^{\rm int}$ of a quantity of interest $\mathcal{O} = \langle\overline{\mathcal{O}}\rangle$ with $\overline{\mathcal{O}} = (1/N_m)\sum_{i=1}^{N_m}\mathcal{O}_i$ and $\mathcal{O}_i$ computed for each path $i$ in the sample. It enters the statistical error estimate $\Delta_{\mathcal{O}}$ for expectation values of $\mathcal{O}$ computed from a Monte Carlo sample of $N_m$ autocorrelated configurations as

$$\Delta\overline{\mathcal{O}} = \sqrt{\frac{\sigma_{\mathcal{O}_i}^2}{N_m}}\sqrt{2\tau_{\mathcal{O}}^{\rm int}}, \tag{7}$$

where $\sigma_{\mathcal{O}_i}^2$ is the variance of $\mathcal{O}_i$.

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With Monte Carlo generated samples of Feynman paths one can thus "measure" thermodynamic properties of quantum systems like the internal energy and the specific heat, but also gain more detailed information about correlation functions, probability distributions and the like. In the low-temperature limit, $\beta \to \infty$, quantum mechanical ground-state properties are recovered.

## 3 Blazing Trails

A pioneer in the application of the Monte Carlo method to physics problems, notably by applying it to the Ising model, was Lloyd D. Fosdick. He appears to have also been one of the first to consider the stochastic sampling of paths. In 1962, he considered the possibility of sampling paths [6] for what he called the conditional Wiener integral, i.e. the Wiener integral for fixed end points. As a toy example he investigated the expectation value of the functional $\exp\left[-\int_0^1 \int_0^1 \tau\tau' x(\tau)x(\tau')d\tau d\tau'\right]$ for a conditional Wiener process, and, more generally, for the quantity $\exp\left[-\int_0^\beta V(x(\tau))d\tau\right]$, i.e. he considered direct computation of the partition function for a quantum particle moving in a potential $V$. He introduced a Fourier decomposition of the paths and generated these by direct Monte Carlo sampling of the Fourier components as Gaussian stochastic variables. He did some explicit sampling of his toy model to demonstrate the feasibility of the method, but a theoretical consideration of the one-dimensional harmonic oscillator was not considered worthwhile to be put on the computer, even though Fosdick, at the time, was at the University of Illinois and had access to the university's ILLIAC computer. His examples were primarily used to investigate the principle feasibility and possible accuracy obtainable by the method. Instead, Fosdick studied a pair of two identical particles and presented some numerical results for this problem. Continuation of the work on the two-particle problem together with a graduate student led to the publication of a paper on the Slater sum, i.e. the diagonal density matrix elements, for $^4$He in 1966 [7], and on three-particle effects in the pair distribution function for $^4$He in 1968 [8]. In the same year [9], Fosdick elaborated on the numerical method in a report on the Monte Carlo method in quantum statistics in the SIAM review. Instead of sampling the Fourier components he now used the discrete time approximation of the paths. Sampling of $x_i$ at the discrete points was done using a trick that later would gain prominence in PIMC simulations in an algorithm called staging. The

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idea was to express the discretized kinetic term in the relative probability density $p(x_i|x_{i-1},x_{i+1}) = (1/2\pi\epsilon)\exp\left[-(x_i-x_{i-1})^2/2\epsilon-(x_{i+1}-x_i)^2/2\epsilon\right]$ as $-(x_i-\bar{x}_i)^2/2\sigma^2+(x_{i-1}-x_{i+1})^2/4\epsilon$ with $\bar{x}_i=(x_{i-1}+x_{i+1})/2$ and to sample $(x_i-\bar{x}_i)/\sigma$ as an independent Gaussian variable. The procedure could be iterated recursively for all $x_i$ and thus allowed to obtain statistically independent paths which were used to "measure" the potential energy term $\exp\left[-\int_0^\beta V(x(\tau))d\tau\right]$.

In 1969, Lawande, Jensen, and Sahlin introduced Metropolis sampling of paths in discrete time, broken line approximation [10]. They investigated the ground-state wave functions of simple one-dimensional problems (harmonic oscillator, square well, and Morse potential) and, theoretically, also addressed the problem of extracting information about excited energies and of simulating many particle problems. In a follow-up paper [11] they presented studies of the Coulomb problem using Monte Carlo simulations of the path integral in polar coordinates. Not surprisingly, the singularity at the origin had to be avoided by artificial constraints and the authors admitted that a more rigorous justification of their procedure was called for. The path integral was later solved exactly by Duru and Kleinert in 1979 [12]. It became clear that there were fundamental problems with such singularities in time-sliced path integrals [2].

Little activity is recorded in the seventies, and I am only aware of a brief theoretical consideration of the possibility of Monte Carlo sampling of paths in a paper by Morita on the solution of the Bloch equation for many particle systems in terms of path integrals from 1973 [13]. The paper is cited in a later one by J.A. Barker published in 1979 [14] in which the one-dimensional particle in a box is considered, and numerical estimations of the ground-state energy and wave function are presented. The data were obtained by introducing image sources to take account of the boundary conditions of the box and using Metropolis sampling of the broken line approximation of the paths. Incidentally, the analytic solution of this problem, i.e. of the path integral for the particle in the box was given by Janke and Kleinert almost simultaneously [15]. Barker also computed distribution functions for the problem of two particles in a box.

Very much in the spirit of Lawande *et al.*, but possibly unaware of this work, Creutz and Freedman published a didactic paper on *a statistical approach to quantum mechanics* in 1981 [16]. They, too, performed Metropolis sampling of paths in the broken line approximation and studied the energies

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and ground-state wave functions of the one-dimensional harmonic oscillator. The background of these authors were Monte Carlo studies of gauge field theories, and the paper was meant as an attempt to better understand the Monte Carlo method by applying it to simple one-degree-of-freedom Schrödinger problems. It still is a useful introduction to the basics of the technique, and in particular, it presents a brief primer on the theory of Markov chains underlying the Metropolis algorithm. To compute energies, they introduced an alternative estimator by invoking the virial theorem. They also studied double-well problems, presenting snap shot pictures of double-kink instanton paths. The problem of determining the energy level splitting was addressed by computing correlation functions.

The papers by Lawande *et al.* and by Creutz and Freedman appear to have been cited very rarely, possibly because they presented their work as being only of pedagogic value and not so much because the Monte Carlo method could be a useful method to obtain numerical results for Schrödinger problems which, in real life, should be handled by numerical methods more suitable in this simple case. These remarks also hold for work published a little later by Shuryak [17,18].

Fosdick's work from 1962 was done very much at the forefront of the technological possibilities of high-speed computing at the time. By the mid-eighties, path-integral simulations of simple quantum mechanical problems had become both conceptually and technically "easy". Indeed, the exposition by Creutz and Freedman was already written in an introductory, didactic manner, and in 1985 the simulation of the one-particle harmonic oscillator was explicitly proposed as an undergraduate project, to be handled on a Commodore CBM3032 microcomputer, in a paper published in the American Journal of Physics [19].

## 4 Speeding Up

The feasibility of evaluating the quantum statistical partition function of many-particle systems by Monte Carlo sampling of paths was well established in the early eighties and the method began to be applied to concrete problems, in particular in the chemical physics literature. It had also become clear that the method had severe restrictions if numerical accuracy was called for. In addition to the statistical error inherent to the Monte Carlo method, a systematic error was unavoidably introduced by the necessary discretization of the paths. Attempts to improve the accuracy by algorithmic improvements

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to reduce both the systematic and the statistical errors were reported in subsequent years. The literature is abundant and rather than trying to review the field I shall only indicate some pertinent paths of development.

In Fourier PIMC methods, introduced in 1983 in the chemical physics context by Doll and Freeman [20,21], the systematic error arises from the fact that only a finite number of Fourier components are taken into account. Here the systematic error could be reduced by the method of partial averaging [22,23].

In discrete time approximations arising from the short-time propagator or, equivalently, the high-temperature Green's function, various attempts have been made to find more rapidly converging formulations. Among these are attempts to include higher terms in an expansion of the Wigner-Kirkwood type, i.e. an expansion in terms of $\hbar^2/2m$. Taking into account the first term of such an expansion would imply to replace the potential term $\epsilon V(x_{j-1})$ in (4) by [24-26]

$$\epsilon V(x_{j-1}) \to \frac{\epsilon}{x - x'} \int_x^{x'} dy V(y). \tag{8}$$

This improves the convergence of the density matrix (4) (from even less than $\mathcal{O}(1/L)$) [24] to $\mathcal{O}(1/L^2)$. For the full partition function, the convergence of the simple discretization scheme is already of order $\mathcal{O}(1/L^2)$: due to the cyclic property of the trace, the discretization $\epsilon V(x_{j-1})$ is then equivalent to a symmetrized potential term $\epsilon(V(x_{j-1})+V(x_j))/2$. The convergence behavior of these formulations follows from the Trotter decomposition formula,

$$e^{-(A+B)} = \left[e^{-\frac{A}{L}} e^{-\frac{B}{L}}\right]^L + \mathcal{O}(1/L) = \left[e^{-\frac{A}{2L}} e^{-\frac{B}{L}} e^{-\frac{A}{2L}}\right]^L + \mathcal{O}(1/L^2), \tag{9}$$

valid for non-commuting operators $A$ and $B$ in a Banach space [27], identifying $A$ with the kinetic energy $\beta \sum \hat{\vec{p}}_i^{\,2}/2m_i$ and $B$ with the potential energy $\beta V(\{\hat{x}_i\})$. More rapidly converging discretization schemes were investigated on the basis of higher-order decompositions. Unfortunately, a direct "fractal" decomposition [28] of the form

$$e^{-(A+B)} = \lim_{L\to\infty} \left[e^{\alpha_1 \frac{A}{L}} e^{\beta_1 \frac{B}{L}} e^{\alpha_2 \frac{A}{L}} e^{\beta_2 \frac{B}{L}} \dots\right]^L, \quad \sum \alpha_i = \sum \beta_i = 1 \tag{10}$$

inevitably leads to negative coefficients for higher decompositions [29] and is therefore not amenable to Monte Carlo sampling of paths [30]. Higher-order Trotter decomposition schemes involving commutators have proven to

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be more successful [31-34]. In particular, a decomposition of the form

$$\mathcal{Z} = \lim_{L\to\infty} \mathrm{Tr}\left[e^{-\frac{A}{2L}} e^{-\frac{B}{2L}} e^{-\frac{[[B,A],B]}{24L^3}} e^{-\frac{B}{2L}} e^{-\frac{A}{2L}}\right]^L , \tag{11}$$

derivable by making use of the cyclic property of the trace, is convergent of order $\mathcal{O}(1/L^4)$ and amounts to simply replacing the potential $\epsilon V$ in (4) by an effective potential [32]

$$V_{\text{eff}} = V + \frac{(\beta\hbar)^2}{24mL^2}(V')^2. \tag{12}$$

Another problem for the numerical accuracy of PIMC simulations arises from the analog of the "critical slowing down" problem which is well known for local update algorithms at second-order phase transitions in the simulation of spin systems and lattice field theory. Since the correlations $\langle x_j x_{j+k}\rangle$ between variables $x_j$ and $x_{j+k}$ in the discrete time approximation only depend on the temperature and on the gaps between the energy levels and not, or at least not appreciably, on the discretization parameter $\epsilon$, the correlation length $\zeta$ along the discretized time axis always diverges linearly with $L$ when measured in units of the lattice spacing $\epsilon$. Hence in the continuum limit of $\epsilon \to 0$ with $\beta$ fixed or, equivalently, of $L \to \infty$ for local, importance sampling update algorithms, like the standard Metropolis algorithm, a slowing down occurs because paths generated in the Monte Carlo process become highly correlated. Since autocorrelation times diverge in simulations using the Metropolis algorithm as [35] $\tau_{\mathcal{O}}^{\text{int}} \propto L^z$ with $z \approx 2$, the computational effort (CPU time) to achieve comparable numerical accuracy in the continuum limit $L \to \infty$ diverges as $L \times L^z = L^{z+1}$.

To overcome this drawback, ad hoc algorithmic modifications like introducing collective moves of the path as a whole between local Metropolis updates were introduced then and again. One of the earliest more systematic and successful attempts to reduce autocorrelations between successive path configurations was introduced in 1984 by Pollock and Ceperly [36]. Rewriting the discretized path integral, their method essentially amounts to a recursive transformation of the variables $x_i$ in such a way that the kinetic part of the energy can be taken care of by sampling direct Gaussian random variables and a Metropolis choice is made for the potential part. The recursive transformation can be done between some fixed points of the discretized paths, and the method has been applied in such a way that successively finer discretizations of the path were introduced between neighbouring points. Invoking the poly-

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mer analog of the discretized path this method was christened the "staging" algorithm by Sprik, Klein, and Chandler in 1985 [37].

The staging algorithm decorrelates successive paths very effectively because the whole staging section of the path is essentially sampled independently. In 1993, another explicitly non-local update was applied to PIMC simulations [35,38] by transferring the so-called multigrid method known from the simulation of spin systems. Originating in the theory of numerical solutions of partial differential equations, the idea of the multigrid method is to introduce a hierarchy of successively coarser grids in order to take into account long wavelength fluctuations more effectively. Moving variables of the coarser grids then amounts to a collective move of neighbouring variables of the finer grids, and the formulation allows to give a recursive description of how to cycle most effectively through the various levels of the multigrid. Particularly successful is the so-called W-cycle. Both the staging algorithm and the multigrid W-cycle have been shown to beat the slowing down problem in the continuum limit completely by reducing the exponent $z$ to $z \approx 0$ [39].

Another cause of severe correlations between paths arises if the probability density of configurations is sharply peaked with high maxima separated by regions of very low probability density. In the statistical mechanics of spin systems this is the case at a first-order phase transition. In PIMC simulations the problem arises for tunneling situations like, e.g. for a double-well potential with a high potential barrier between the two wells. In these cases, an unbiased probing of the configuration space becomes difficult because the system tends to get stuck around one of the probability maxima. A remedy to this problem is to simulate an auxiliary distribution that is flat between the maxima and to recover the correct Boltzmann distribution by an appropriate reweighting of the sample. The procedure is known under the name of umbrella sampling or multicanonical sampling. It was shown to reduce autocorrelations for PIMC simulations of a single particle in a one-dimensional double well, and it can also be combined with multigrid acceleration [40].

The statistical error associated with a Monte Carlo estimate of an observable $\mathcal{O}$ cannot only be minimized by reducing autocorrelation times $\tau_{\mathcal{O}}^{\mathrm{int}}$. If the observable can be measured with two different estimators $U_i$ that yield the same mean $U_i^{(L)} = \langle U_i \rangle$ with $\mathcal{O} = \lim_{L\to\infty} U_i^{(L)}$, the estimator with the smaller variance $\sigma_{U_i}^2$ is to be preferred. Straightforward differentiation of the discretized path integral (4) leads to an estimator of the energy that explicitly

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measures the kinetic and potential parts of the energy by

$$U_{\rm k} = \frac{L}{2\beta} - \frac{m}{2L}\sum_{j=1}^{L}\left(\frac{x_j - x_{j-1}}{\epsilon}\right)^2 + \frac{1}{L}\sum_{i=1}^{L} V(x_i). \tag{13}$$

The variance of this so-called "kinetic" energy estimator diverges with $L$. Another estimator can be derived by invoking the path-integral analog of the virial theorem

$$\frac{L}{2\beta} - \frac{m}{2}\left\langle\left(\frac{x_j - x_{j-1}}{\epsilon}\right)^2\right\rangle = \frac{1}{2}\langle x_j V'(x_j)\rangle, \tag{14}$$

and the variance of the "virial" estimator

$$U_{\rm v} = \frac{1}{2L}\sum_{i=1}^{L} x_i V'(x_i) + \frac{1}{L}\sum_{i=1}^{L} V(x_i) \tag{15}$$

does not depend on $L$. In the early eighties, investigations of the "kinetic" and the "virial" estimators focussed on their variances [32,41,42]. Some years later, it was pointed out [43] that a correct assessment of the accuracy also has to take into account the autocorrelations, and it was demonstrated that, for a standard Metropolis simulation of the harmonic oscillator, the allegedly less successful "kinetic" estimator gave smaller errors than the "virial" estimator. In 1989 it was shown [44] that conclusions about the accuracy also depend on the particular Monte Carlo update algorithm at hand, since modifications of the update scheme such as inclusion of collective moves of the whole path affect the autocorrelations of the two estimators in a different way. A careful comparison of the two estimators which disentangles the various factors involved was given only quite recently [45]. Here it was also shown that a further reduction of the error may be achieved by a proper combination of both estimators without extra cost.

## 5 Concluding Remarks

The application of the Monte Carlo method to quantum systems is not restricted to direct sampling of Feynman paths, but this method has attractive features. It is not only conceptually suggestive but also allows for algorithmic improvements that help to make the method useful even when the problems at hand require considerable numerical accuracy. However, algorithmic improvements like the ones alluded to above have been proposed and tested

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mainly for simple one-particle systems. On the other hand, the power of the Monte Carlo method is, of course, most welcome in those cases where analytical methods fail. For more complicated systems, however, evaluating the algorithms and controlling the numerical accuracy is also more difficult. Only recently, a comparison of the efficiency of Fourier- and discrete time-path integral Monte Carlo for a cluster of 22 hydrogen molecules was presented [46] and debated [47,48]. Nevertheless, path-integral Monte Carlo simulations have become an essential tool for the treatment of strongly interacting quantum systems, like, e.g. the theory of condensed helium [49].

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