Acknowledgments
We acknowledge financial support from the Ministry of Science and Environmental Protection of the Republic of Serbia through Projects No. 1486, No. 1899, and No. 141035.

References

1. A. Balaž, A. Belić, and A. Bogojević, Phys. Low-Dim. Struct. 7/8, 33 (2002).
2. R. P. Feynman and A. R. Hibbs, Quantum Mechanics and Path Integrals, McGraw-Hill, New York, 1965.
3. H. Kleinert, Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets, World Scientific, Singapore, 2004.
4. A. Balaž, A. Belić, and A. Bogojević, SFIN A2, 297 (1998); Phys. Low-Dim. Struct. 5/6, 1 (1999); ibid. 9/10, 149 (1999); ibid. 12, 65 (2000); ibid. 7/8, 121 (2000); ibid. 9/10, 113 (2000).
5. M. H. Kalos and P. A. Whitlock, Monte Carlo methods, Volume 1: Basics, John Wiley and Sons, New York, 1986.
6. W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, Numerical Recipes in C: The Art of Scientific Computing, Cambridge University Press, Cambridge, UK, 1992.

Поступила в редакцию 25.04.2005 (Received 25.04.2005)

Linearized Gaussian Halving in *d*=1

A.Bogojević, A.Balaž, and A.Belić*
Scientific Computing Laboratory Institute of Physics

**abelic@phy.bg.ac.yu*

We present an extension of a new Gaussian halving method for the calculation of path integrals introduced in Refs. [1-3]. The original method leads to recursion relations that are nonlinear and could not be solved analytically. In this paper we present a general analytical solution (including the continuum limit) of linearized recursions. We show that the error associated with this linearization is of the order $O(1/N^2)$, where N is the number of discretized steps, i.e. it is of the same order of magnitude as the error inherent in the derivation of the original method. Using this result we derive an improved algorithm for calculation of path integrals.

1. Linearized Recursion

In a series of previous papers [1-4] we have shown that in the case of quantum theories described by Hamiltonians of the form $H = \frac{1}{2} G(q)\dot{q}^2 + V(q)$ the solution of the associated path integral can be substantially sped up through iterating the recursion relation

$$G_s^{(k+1)} = \mathrm{G}\left[G_s^{(k)}, V_s^{(k)}, \frac{\varepsilon_N}{2^{s-k-1}} \right], \tag{1}$$

$$V_s^{(k+1)} = \mathrm{V}\left[G_s^{(k)}, V_s^{(k)}, \frac{\varepsilon_N}{2^{s-k-1}} \right], \tag{2}$$

where s is any positive integer, $k = 0, 1, 2, \ldots, s$, and functions G and V are given by

$$\mathrm{G}[G, V, \varepsilon_N] = G - \frac{\varepsilon_N}{16}\left[\frac{G''}{G} - \left(\frac{G'}{G} \right)^2 \right] + \frac{\varepsilon_N^2}{16} V'', \tag{3}$$

$$\mathrm{V}[G, V, \varepsilon_N] = V + \frac{1}{\varepsilon_N}\ln\frac{\mathrm{G}}{G} - \frac{\left(\frac{G'}{G} - \varepsilon_N V'\right)^2}{32\,\mathrm{G}}. \quad (4)$$

The above recursion relations link different discretizations of the same theory. In the case of N slices the minimal discretization step is given by $\varepsilon_N = \beta / N$, where β denotes the inverse temperature. The seed terms in the recursion (corresponding to $k = 0$) are the functions G and V from the starting action S, while the remaining iterates represent corresponding terms for a series of effective actions $S_{N,k}$.

The Gaussian halving method starts from solving the odd numbered integrations in the expression for the generating functional. In this way one obtains a connection between the N-point and $N/2$-point discretizations of the theory. The aforementioned integrations are calculated through an analytical approximation that casts them in the form of Gaussian integrals. This is done by expanding the discretized action in the mid-point prescription up to quadratic terms in the differences $q_{i+1} - q_i$. We have shown [1, 2] that by the recursive application of this halving scheme we end up with an error proportional to $1/N^2$, i.e. an error that is subdominant with respect to the standard expansion of Z_N about its continuum limit [5, 6], which is of the form $Z_N = Z + a/N + b/N^2 + O(1/N^3)$. Note that equations (1-4) drive the Gaussian halving procedure from an initial discretization with $2^s N$ slices ($k = 0$) to a final discretization with N slices ($k = s$).

It was also shown [2] that by using the effective action $S_{N,k}$ instead of the original action S one finds $Z_{N,k} = Z + a'/2^k N + b'/N^2 + O(1/N^3)$. The crucial thing to note is that in both expansions one is dealing with the same continuum value Z. In addition, both continuum expansions are given in terms of the same coefficient a. As a result of this we see that it is best to start with as high an iterate in the recursion relation for the effective action as possible as this decreases the error. Ideally we should use the continuum limit of the recursion (set $k = s$ and take the limit $s \to \infty$) as this would eliminate the dominant $O(1/N)$ term in the above expansion and would lead to a much smaller error.

The nonlinearity of the recursion relations, however, makes it impossible to obtain an analytical solution. In this paper we will linearize the Gaussian halving recursion relations and will present a general solution of those relations. Let us note that for short time of propagation the generic theory obeys $(q_{i+1} - q_i)^2 \propto \varepsilon_N$. This means that the original recursion relations can be linearized (through an expansion in ε_N) without introducing a significant new coarsening of our method. A straightforward linearization gives us

$$G_s^{(k+1)} = G_s^{(k)} + \frac{\varepsilon_N^2}{16}\frac{V_s^{(k)\prime\prime}}{2^{2s-2k-2}} - \frac{\varepsilon_N}{16}\frac{G_s^{(k)\prime\prime}}{2^{s-k-1}}, \quad (5)$$

$$V_s^{(k+1)} = V_s^{(k)} + \frac{\varepsilon_N}{16}\frac{V_s^{(k)\prime\prime}}{2^{s-k-1}}. \quad (6)$$

We note that the V's and G's are expanded to different powers in ε_N since in the expression for the discretized action the potential term is multiplied by ε_N, while the kinetic term is multiplied by $1/\varepsilon_N$. The linearized recursions are easily solved. The solution for the theories with $G = 1$ in the original action (the majority of theories of interest) is

$$G_s^{(k)} = 1 + \frac{4^k - 1}{12 \cdot 4^s} \varepsilon_N^2 V_0'' + \frac{2 \cdot 8^k - 7 \cdot 4^k + 7 \cdot 2^k - 2}{672 \cdot 8^s} \varepsilon_N^3 V_0'''', \quad (7)$$

$$V_s^{(k)} = V_0 + \frac{2^k - 1}{8 \cdot 2^s} \varepsilon_N V_0'' . \quad (8)$$

In passing, let us note that the Gaussian halving method guarantees that all the effective actions remain of the same general form as the starting action (in particular, they are all quadratic in velocities). However, as we can see, the effective actions will acquire non-trivial kinetic terms ($G \neq 1$) even if the starting action has a trivial kinetic term.

On the basis of the above general solution we easily find the thing that interests us most - the continuum limit of the effective action recursions. This is just the $s \to \infty$ limit of the above expressions for $G_s^{(s)}$ and $V_s^{(s)}$, i.e.

$$G_\infty^{lin} = \lim_{s \to \infty} G_s^{(s)} = 1 + \varepsilon_N \frac{V_0''}{12} + \varepsilon_N^3 \frac{V_0''''}{336}, \quad (9)$$

$$V_\infty^{lin} = \lim_{s \to \infty} V_s^{(s)} = V_0 + \varepsilon_N \frac{V_0''}{8} . \quad (10)$$

2. Numerical results

We have tested the validity of the obtained analytical results on a broad slice of parameter space of a harmonic oscillator with quartic anharmonicity, including very large values of coupling (e.g. $g = 100$) and of inverse temperature β. All the results were obtained through the use of numerical Monte Carlo simulations [7]. Fig. 1 shows the error brought in by linearization. The deviations from the solutions of the original Gaussian halving

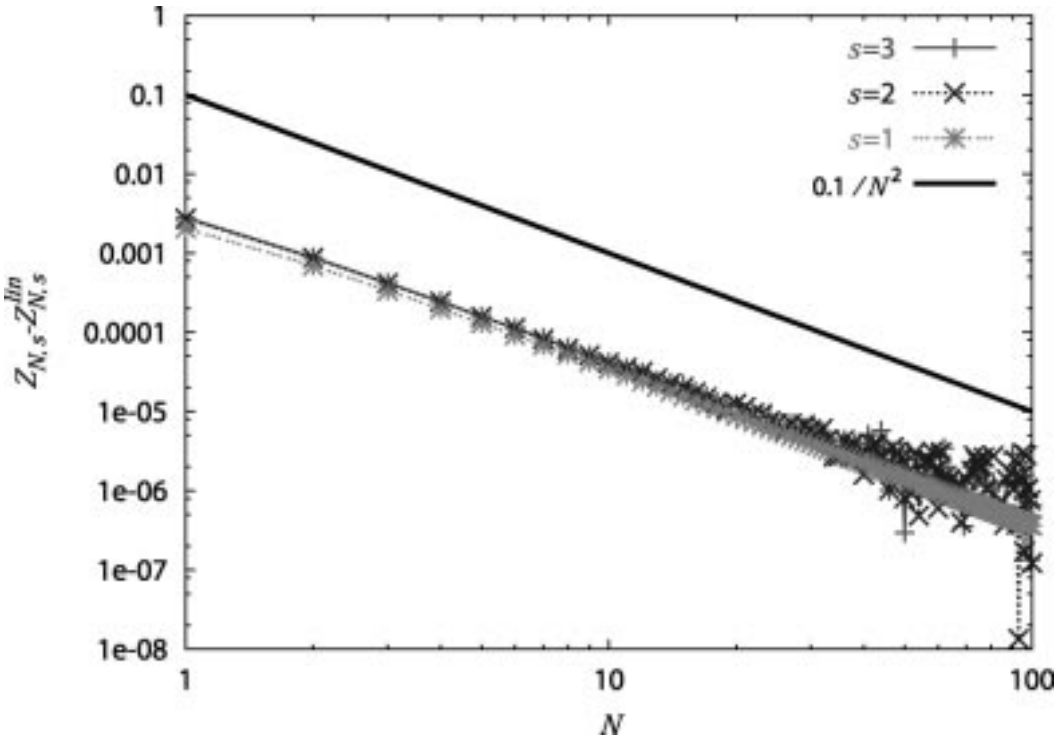

Fig. 1. The error brought in by linearizing as a function of N. 1/N² dependence is illustrated by plotting the curve 0.1/N². The parameters of the theory: g = 1, β = 1, number of Monte Carlo steps

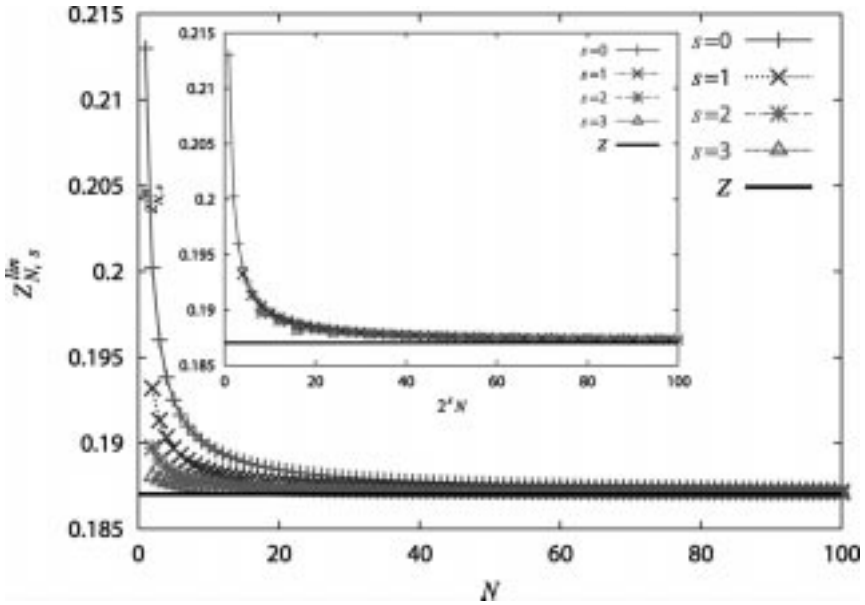

Fig. 2. $Z^{lin}_{N,s}$ ***as a function of the number of discretized time steps N. The parameters of the theory:*** $g = 1$, $\beta = 1$, $N_{MC} = 10^7$. ***The inset graph shows that the effective actions calculated from the linearized theory lead to the same kind of scaling as do the solutions of the original Gaussian halving recursion (i.e. all the N and s dependence of these generating functionals is combined in a single parameter*** $N_{eff} = 2^s N$ ***)***

recursion relations is of order $O(1/N^2)$, i.e. it is of the same order of magnitude as the error associated with the Gaussian halving method itself.

As a result of this we can calculate path integrals by using the analytically calculated expressions for the effective actions obtained through the solution of the linearized recursions. Fig. 2 shows how $Z^{lin}_{N,s}$ converges to the same continuum limit as the original action, only faster. The inset plot shows that the linearized expressions display the same scaling as the original expressions, i.e. that all the $Z^{lin}_{N,s}$ collapse to a single curve depending only on $N_{eff} = 2^s N$.

A more detailed numerical investigation shows that for the $Z^{lin}_{N,s}$ we have the following behavior: $Z^{lin}_{N,s} = Z + a/2^s N + b''/N^2 + O(1/N^3)$. The dominant $O(1/N)$ term remains the same as in the original Gaussian halving (since the error associated with linearization is of order $O(1/N^2)$). What has changed is the coefficient of the subdominant term. Unlike the case of the original Gaussian halving recursions, here we can do the limit $s \to \infty$. Fig. 3 shows that by doing this we really do get rid of the dominant term in expansion of the partition function. As we have already indicated, by using $Z^{lin}_{N,\infty}$ for calculating the path integral of the generating functional we make an error that is of order $O(1/N^2)$. From the above plot we see that this new calculation scheme gives excellent results even for extremely coarse discretizations, i.e. for very small values of N.

In the language of numerical simulations this can be stated in another way - the continuum limit of linearized Gaussian halving leads to a vast speed-up in the algorithm for the calculating of generic path integrals (several thousand fold speed-up for typical precisions, and a much greater speed-up in the case of high precision path integral calculations).

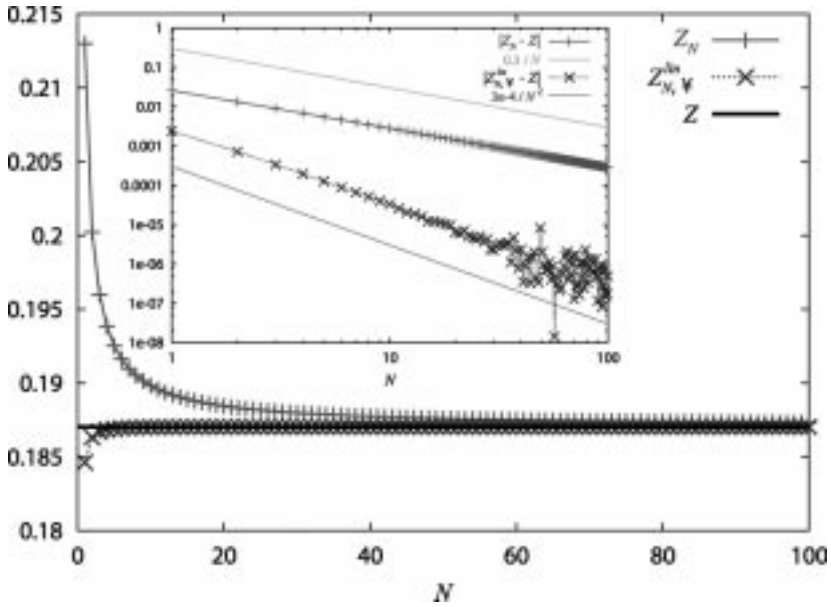

Fig. 3. Comparison of how Z_N ***(standard algorithm for calculating path integrals) and*** $Z^{lin}_{N,\infty}$ ***(new algorithm) tend to the continuum value Z. The parameters of the theory:*** $g=1$, $\beta=1$, $N_{MC}=10^7$. ***The inset plot shows that the new algorithm has an error of order O(1/N [2]), while the error in the standard algorithm is of order O(1/N)***

3. Conclusion

In this paper we have presented the linearization of recently developed recursion relations for path integrals [1-4]. We have analytically solved these linearized relations for the case of a general theory (including the continuum limit) and have shown that the error due to linearization is of the order $O(1/N^2)$, the same order as the error inherent in the method of Gaussian halving. Using this we have presented a generic algorithm for calculating path integrals that is far more efficient than the standard one: for the same time of calculation the standard algorithm leads to an error that is of order $O(1/N)$, while the new algorithm has a total error proportional to $1/N^2$. Alternately, for a given precision, the new algorithm leads to a vast speed-up in the time needed to calculate a generic path integral.

We acknowledge financial support from the Ministry of Science and Environmental Protection of the Republic of Serbia through Projects No. 1486, No. 1899, and No. 141035.

References

1. A.Balaž, A.Belić, and A.Bogojević, submitted to Phys. Low-Dim. Struct. 1, 49 (2006).

2. A.Balaž, A.Belić, and A.Bogojević, in Proceedings of the XI Congress of Physicists of Serbia and Montenegro 5, 169 (2004); ibid. 5, 173 (2004); ibid. 5, 177 (2004).

3. A.Balaž, A.Belić, and A.Bogojević, Phys. Low-Dim. Struct. 7/8, 33 (2002).

4. A.Balaž, A.Belić, and A.Bogojević, SFIN A2, 297 (1998); Phys. Low-Dim. Struct. 5/6, 1 (1999); ibid. 9/10, 149 (1999); ibid. 12, 65 (2000); ibid. 7/8, 121 (2000); ibid. 9/10, 113 (2000).

5. R.P.Feynman and A.R.Hibbs, Quantum Mechanics and Path Integrals, McGraw-Hill, New York, 1965.

6. H. Kleinert, Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets, World Scientific, Singapore, 2004.

7. M.H.Kalos and P. A. Whitlock, Monte Carlo methods, Volume 1: Basics, John Wiley and Sons, New York, 1986.