New enhancements to Feynman's Path Integral for fermions

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Abstract

We show that the computational effort for the numerical solution of fermionic quantum systems, occurring e.g., in quantum chemistry, solid state physics, field theory in principle grows with less than the square of the particle number for problems stated in one space dimension and with less than the cube of the particle number for problems stated in three space dimensions. This is proven by representation of effective algorithms for fermion systems in the framework of the Feynman Path Integral.
I. INTRODUCTION

When Feynman stated the thermodynamical Path Integral for fermions (see \cite{1} and references therein), he was in doubt whether this formula could ever be used in numerical applications. However, in the last few years considerable progress has been made in the development of Path Integral Monte Carlo algorithms. Especially D. Ceperly et. al. \cite{2} proposed many very useful refinements. Nevertheless, the problem of applying Path Integral methods to fermion systems remains hard to be solved. The reasons are the so-called fermion sign problem and the computational effort, which grows normally proportional to the fourth power of the number of particles \( N \). In this letter we present a formally exact method with a computational effort growing only with the cube of the particle number. We further show, that there are some strong indications, that the computational effort should in general grow only with the square of the particle number. For problems stated in one space dimension, we give an explicit proof for that.

II. EFFECTIVE PATH INTEGRAL METHOD

A quantum \( N \) body system in thermal equilibrium can be described completely by the quantum partition function

\[
Z = \text{Tr} \exp(-\beta(H_0 + H_1)),
\]

where \( H_0 \) and \( H_1 \) are the kinetic and potential energy operator. The Path Integral formalism leads to a computational convenient equation to calculate \( Z \). Using Trotter’s formula \cite{3} \( Z \) can be approximated by

\[
Z = \text{Tr} \left( \exp(-\frac{\beta}{M}H_0)\exp(-\frac{\beta}{M}H_1) \right)^M + O(\beta^3/M^2).
\]

For a system of polarized fermions in \( d \) space dimensions this leads to the \( dNM \) dimensional integral:
$$Z = \left( \frac{1}{N!} \right)^M \int \prod_{i=1}^{M} \prod_{\gamma=1}^{N} d\vec{x}_i(\gamma) \prod_{\delta=1}^{M} \det A(\delta + 1, \delta) \exp \left( -\frac{\beta}{M} \sum_{\alpha=1}^{M} V(\vec{x}_1(\alpha), \ldots, \vec{x}_N(\alpha)) \right),$$  \hspace{1em} (3)

with

$$\langle A(\alpha + 1, \alpha) \rangle_{k,l} = \left( \frac{Mm}{2\pi\beta\hbar^2} \right)^{d/2} \exp \left( -\frac{Mm}{2\beta\hbar^2} (\vec{x}_k(\alpha + 1) - \vec{x}_l(\alpha))^2 \right),$$  \hspace{1em} (4)

and the periodicity condition $\vec{x}_i(M + 1) = \vec{x}_i(1)$. The particle mass is denoted by $m$.

A number of useful modifications to (3), which improve the convergence vs. the number of timesteps $M$ (see e.g. [4,5]), are known. Because these modifications do not affect any of the following we will not stress them here.

Usually the Metropolis algorithm [6] is adopted to evaluate (3). The improvements presented in this paper are based on a careful analysis of the numerical algorithms.

Within the Metropolis Monte Carlo procedure a Markov process has to be generated, under which the probability distribution is stationary. In our case this condition is fulfilled by the following widely used procedure, in which the sampling of the probability distribution is done by generating two different types of random moves of the particle coordinates.

In every microscopic step, all time slices of all particle coordinates are moved separately through

$$\vec{x}_i(\alpha) \rightarrow \vec{x}_i(\alpha) + \Delta\vec{x},$$  \hspace{1em} (5)

where $\Delta\vec{x}$ is a randomly chosen vector. In every macroscopic step all time slices of every particle coordinate are moved at once by constant vector.

$$\vec{x}_i(\alpha) \rightarrow \vec{x}_i(\alpha) + \Delta\vec{y}, \quad \alpha = 1 \ldots M.$$  \hspace{1em} (6)

In both cases a move is accepted, if the absolute value of the ratio of weight functions, which are simply the integrands in (3), is greater than a homogeneous random number. Here it is important that the absolute values have to be taken, because the determinant occurring in the weight function $W(p)$ becomes sometimes negative.

Any observable $X$ can then be evaluated through
\[
\langle X \rangle = \frac{\sum_{p=1}^{G} X(p) \text{sign}(W(p))}{\sum_{p=1}^{G} \text{sign}(W(p))}
\]

where the summation in (7) runs over all Metropolis steps, \(X(p)\) being the value of \(X\) in the \(p\)-th step.

Albeit the fact, that this method has been applied in some cases (see e.g. [7]), its usefulness is limited by its high computational costs. The main effort in the numerical computation of (3) is the calculation of the determinant. In every complete microscopic motion the determinant has to be calculated \(N \times M\) times. The complete algorithm is therefore of order \(\leq N^4\), if standard matrix factorizations, which are of order \(N^3\), are used. The lower sign stands, because we found that the number of iterations necessary to achieve a given precision in the numerical solution decreases with an increasing number of particles. This results simply from the fact that a larger number of identical particles yields better statistics.

Now observe, that every change of a microscopic coordinate affects only the \(i\)'th row of matrix \(A(\alpha + 1, \alpha)\) and the \(i\)'th column of matrix \(A(\alpha, \alpha - 1)\). This simple fact can be used to reduce the numerical effort by a factor \(n\). The reason for that is that the updating of an \(LU\) factorization of a matrix after a row or column exchange can be done by a numerical effort proportional to \(N^2\). Descriptions of such algorithms can be found in some textbooks on matrix computations [8]. We thus claim that the total algorithm is only of order \(N^3\).

Encouraged by the above result and through the fact that the matrix (4) has some hidden symmetries having only \(2dN\) independent parameters instead of \(N^2\), we found for the special case of systems describable in one space dimension \((d = 1)\) a further reduction of the numerical effort.

Absorbing the trivial constant factors in (4) the problem is reduced to calculate the determinant of matrices of the form

\[
B_{i,j} = \exp\left(-\frac{1}{2}(x_i - y_j)^2\right).
\]

Using the linear properties of \(\det\) we have
\[
\det(B) = \det(M) \prod_{j=1}^{N} \exp\left(-\frac{1}{2}(x_j^2 + y_j^2)\right).
\] (9)

We now show, that the determinant of matrices of the special form
\[
M_{i,j} = \exp(x_i y_j)
\] (10)
can be calculated with an effort of only \(N^2\) operations. This can most easily be seen using the decomposition \(M = RST\) of (10).

\[
R = \begin{pmatrix}
1 & y_1 & y_1^2 & \cdots \\
1 & y_2 & y_2^2 & \cdots \\
\vdots & \vdots & \vdots \\
1 & y_N & y_N^2 & \cdots
\end{pmatrix},
\quad
S = \begin{pmatrix}
0! & 0 & 0 & \cdots \\
0 & 1! & 0 & \cdots \\
0 & 0 & 2! & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix},
\quad
T = \begin{pmatrix}
x_1 & x_2 & \cdots & x_N \\
x_1^2 & x_2^2 & \cdots & x_N^2 \\
\vdots & \vdots & \vdots & \vdots
\end{pmatrix}.
\] (11)

The truncation of these infinite matrices to simple \((N \times N)\)-matrices corresponds to a truncation of the exponential series at order \(N - 1\). For sufficiently large \(N\) there is obviously no problem in doing so and we have
\[
\det(M) = \det(R) \det(S) \det(T).
\] (12)

The calculation of \(\det(S)\) is just trivial and yields a constant for given \(N\). \(R\) and \(T\) are Vandermonde matrices, for which the calculation of the determinants is extremely simple [3]. For example for \(R\) we have
\[
\det(R) = \prod_{1 \leq j < i \leq N} (x_i - x_j).
\] (13)

The complete calculation of \(\det M\) thus involves \(N(N - 1)\) subtractions and \(N(N - 1)\) multiplications altogether. Again using the fact, that only one coordinate is changed in one microscopic step, the algorithm to compute the determinant is of order \(N\) and the complete Monte Carlo algorithm thus of order \(N^2\).

Thus we are able to rewrite (3) as
\[
Z = \left(\frac{1}{N!}\right)^M \left(\frac{Mm}{2\pi\beta h^2}\right)^{NM/2} \left(\prod_{i=1}^{N} \frac{1}{i!}\right) \int \prod_{\alpha=1}^{M} \prod_{i=1}^{N} dx_i(\alpha) \exp\left(-\frac{Mm}{\beta h^2} \sum_{\alpha=1}^{M} \sum_{j=1}^{N} x_j^2(\alpha)\right) \left(\frac{Mm}{\beta h^2}\right)^N \left(\prod_{\alpha=1}^{M} \prod_{i<k}^{N} (x_k(\alpha + 1) - x_i(\alpha))^2\right) \exp\left(-\frac{\beta}{M} \sum_{\alpha=1}^{M} V(\vec{x}_1(\alpha), \ldots, \vec{x}_N(\alpha))\right).
\] (14)
III. CONCLUSION

Our almost trivial looking results based on basic linear algebra contribute a significant improvement to the Path Integral method. The decomposition of (10) found together with the truncation of the indefinite matrices is somewhat unsatisfactory, because the method applies in principle only to large particle numbers. Nonetheless our results should be encouraging to continue to look for efficient algorithms to compute the determinant of (10). Because of the equivalence of the mathematical problem, quite generally our result implies that any solution method for quantum systems involving fermions should be bound by a computational effort of order $N^2$. Indeed, a completely different method of computing the Path Integral for $N$ fermion and boson systems was found, which has this property [10,11].
REFERENCES

[1] R.P. Feynman, A.R. Hibbs : Quantum Mechanics and Path Integrals New York: Mc-Graw Hill 1965

[2] D.M. Ceperly, Phys.Rev.Lett. 69, 331 (1992)
   E.L. Pollock, D.M. Ceperly, Phys.Rev. B 30, 2555 (1984)
   E.L. Pollock, D.M. Ceperly, Phys.Rev. B 36, 8343 (1987)

[3] M.F. Trotter , Proc. Am. Math. Soc. 10, 545 (1959)

[4] M. Takahashi, M. Imada , J. Phys. Soc. Jpn. 53, 963 (1984)

[5] M. Takahashi, M. Imada , J. Phys. Soc. Jpn. 53, 3765 (1984)

[6] N. Metropolis, A. Rosenbluth, M.N. Rosenbluth, A.H. Teller, E. Teller , J. Chem. Phys. 21, 1087 (1953)

[7] P. Borrmann, E.R. Hilf, Z.Phys.D 26, S350 (1993)

[8] G.H. Golub, C.F. Van Loan, Matrix Computations, The John Hopkins University Press, Baltimore, Maryland, 1989.
   J.W. Daniel, W.B. Gragg, L. Kaufmann, G.W. Stewart, Mathematics of Computation 30 772 (1976)
   P.E. Gill, G.H. Golub, M. Murray, M.A. Saunders, Mathematics of Computation 28 772 (1976)

[9] R. Bellmann, Introduction to Matrix Analysis, 2nd edition, New Dehli: Tata McGraw-Hill 1979 ( pg. 193 )

[10] P. Borrmann, G.Franke, J.Chem.Phys.98 2484 (1993)

[11] P. Borrmann, Path Integral Density Functional Theory, Preprint UOL-THEO3-94-4, Universität Oldenburg, 1994.