SLAC – PUB – 3788
September 1985
(T)

THE ENSEMBLE PROJECTOR MONTE CARLO METHOD, STUDYING THE LATTICE SCHWINGER MODEL IN THE HAMILTONIAN FORMULATION*

J. RANFT†

Stanford Linear Accelerator Center
Stanford University, Stanford, California, 94305

and

A. SCHILLER

Sektion Physik, Karl-Marx-Universität
Leipzig, G.D.R.

Submitted to *Physical Review D*

* Work supported by the Department of Energy, contract DE – AC03 – 76SF00515.
† Permanent Address: Sektion Physik, Karl-Marx-Universität, Leipzig, G.D.R.

ABSTRACT

The ensemble projector Monte Carlo method is a promising method to study lattice gauge theories with fermions in the Hamiltonian formulation. We study the massive Schwinger model and show, that consistent results are obtained in the presence of positive and negative matrix elements. The expectation values for the average energy calculated from matrix elements with negative and positive scores, and calculated from the average scores are consistent with each other and with results obtained from the local Hamiltonian Monte Carlo method. In contrast to the latter method, the ensemble projector Monte Carlo method can be applied also to gauge field theories in 2+1 and 3+1 dimensions.

1. INTRODUCTION

The introduction of more effective methods for the Monte Carlo simulation of gauge field theories with fermions is an important problem in present day lattice gauge field theories. Most of the Monte Carlo algorithms used at present start from the Wilson formulation of lattice gauge theories.[1] A second method is the Hamiltonian formulation of lattice gauge theories,[2] where the time remains a continuous variable and the formulation is in terms of the lattice Hamiltonian and lattice eigenstates.

The local Hamiltonian Monte Carlo method[3] is an effective Hamiltonian method to treat lattice theories with fermions in $d = 1 + 1$ dimensions. This method was applied to model gauge field theories, like the massless[4] and massive[5] Schwinger model, models with gauge bosons, Higgs bosons and fermions[6] and supersymmetric models.[7] Unfortunately, it is not possible to extend this method to models with more than one spatial dimension.

The projector Monte Carlo method is a new Hamiltonian Monte Carlo method[8] which was applied to lattice models[8] and to pure lattice gauge theories in $d = 2 + 1$ dimensions,[9] to the Schwinger model with fermions[10] and to the $d = 1+1$ SU(2) lattice gauge theory.[11] This method is however rather ineffective especially for large lattices due to the large fluctuations of the scores which go into the calculated expectation values. Because of this, this method was improved in several ways:[8,12–14] The parallel scores method was shown to give good results for the $d = 2 + 1$ U(1) gauge theory without fermions. Another generalization is the ensemble projector method,[13,14] which was applied to the pure U(1) lattice gauge theory in 2+1[15] and 3+1[13] dimensions, to a study of the string tension and of screening in the Schwinger model[16] and to the $d = 1 + 1$ SU(2)-lattice

gauge theory with fermions.[17] Here we continue to study and use this method for the Schwinger model in $d = 1 + 1$ dimensions. the aim of the present paper is, to study the calculation of expectation values with this method in a situation, where matrix elements and scores can have negative signs. This happens in the Schwinger model, if we does not restrict the calculation to lattice configurations periodic in time direction as was done using the local Hamiltonian Monte Carlo method.[3–5]

It was also shown in Ref. 18, that the presence of intrinsic negative signs in the matrix elements does not prevent the Hamiltonian Monte Carlo calculation. The same problem will occur again in Hamiltonian lattice gauge theories with fermions in $d = 2 + 1$ and $d = 3 + 1$ dimensions, which we did start to study.[19]

In Section 2 we present the ensemble projector Monte Carlo method as applied in this paper, in Section 3 we apply the method to the massive Schwinger model. In Section 4 we present and discuss the results.

2. THE ENSEMBLE PROJECTOR MONTE CARLO METHOD

We introduce a lattice Hamiltonian H defined on a discrete spatial lattice, $|\phi\rangle$, $|\psi\rangle$, etc. are lattice eigenstates. The operator $\exp(-\beta H)$ is a projection operator to the lowest energy eigenstate with given quantum numbers.

Provided that $|\chi\rangle$ and $|\phi\rangle$ are states not orthogonal to the lattice ground state $|\psi\rangle$ we calculate expectation values of operators as follows:

$$e^{-\Delta\beta E_0} = \langle e^{-\Delta\beta H}\rangle = \lim_{\beta\to\infty} \frac{\langle\chi|e^{-(\beta+\Delta\beta)H}|\phi\rangle}{\langle\chi|e^{-\beta H}|\phi\rangle} \tag{1}$$

or

$$\langle\psi|Q|\psi\rangle = \lim_{\beta\to\infty} \frac{\langle\chi|e^{-\beta H}\,Qe^{-\beta H}|\phi\rangle}{\langle\chi|e^{-2\beta H}|\phi\rangle} \quad . \tag{2}$$

To calculate the matrix elements in (1) and (2) one splits β in L intercalls $\Delta\tau$

$$\beta = L\,\Delta\tau \tag{3}$$

and furthermore the Hamiltonian into two (one more) parts

$$H = H_1 + H_2 \quad . \tag{4}$$

This splitting is arbitrary provided it leads to local matrix elements down in expression (6) which contain only the variables of one lattice point and its nearest neighbors. We define $U_k = \exp(-\Delta\tau H_k)$ and find

$$e^{-\Delta\tau H} = U_1\,U_2\left(1 - \frac{1}{2}\,\Delta\tau^2\,[H_1, H_2] + \ldots\right) \tag{5}$$

that for sufficiently small $\Delta\tau$ the terms in $\Delta\tau^2$ can be neglected. We obtain for the partition function the expression

$$\begin{aligned} Y(\beta) &= \langle\chi|e^{-\beta H}|\phi\rangle = \langle\chi|\,[U_2\;U_1]^L\,|\phi\rangle \\ &= \sum_{i_{2L+1},i_{2L},\ldots,i_1} \langle\chi|i_{2L+1}\rangle\;\langle i_{2L+1}|U_2|i_{2L}\rangle\;\langle i_{2L}|U_1|i_{2L-1}\rangle\ldots\langle i_2|U_1|i_1\rangle\;\langle i_1|\phi\rangle \end{aligned} \tag{6}$$

where the i_k are complete sets of eigenstates. All matrix elements $\langle i_i|U_k|i_j\rangle$ are local. Each of these matrix elements can be represented as a product of the

probability P_{ij} and the score S_{ij}

$$\langle i_i|U_k|i_j\rangle = P_{ij}(k)\cdot S_{ij}(k) \quad . \tag{7}$$

The $P_{ij}(k)$ are positive definite and normalized

$$\sum_i P_{ij}(k) = 1 \tag{8}$$

but otherwise arbitrary, they should be chosen in such a way that the resulting Monte Carlo method converges optimally. In the projector Monte Carlo method, $P_{ij}(k)$ is used as the probability to sample the slate $|i_i\rangle$ from a given state $|i_j\rangle$ and $S_{ij}(k)$ gives the weight of the state obtained. The result of one iteration starting from a state $|\phi\rangle$ is a sequence of states $i_1, i_2, \ldots, i_{2L+1}$ at different time slices with the weight

$$W\left(i_{2L+1}, i_{2L}, \ldots, i_1\right) = \langle\chi|i_{2L+1}\rangle\ S_{2L+1,2L}\cdot S_{2L,2L-1}\ \ldots\ S_{3,2}\cdot S_{2,1}\ \mathrm{sign}\left(\langle i_1|\phi\rangle\right)\ . \tag{9}$$

For a lattice of large spatial and temporal extension, these weights might fluctuate widely, making the projector Monte Carlo method rather ineffective.

In the ensemble projector method these weight fluctuations are suppressed in the following way. We use an ensemble of say $M = 1000$ lattice states. After each updating of one of these states using the probabilities $P_{ij}(k)$ follows a replication step using the score $S_{ij}(k)$ and some average score S. For

$$q_{ij} = \frac{S_{ij}(k)}{S} \ < \ 1 \tag{10}$$

the given state is retained in the ensemble with the probability q_{ij} or removed with the probability $1 - q_{ij}$. For $q_{ij} = \ell_{ij} + \tilde{q}_{ij} \geq 1$, where ℓ_{ij} is the integer part

of q_{ij}, we add ℓ_{ij} copies of the state to the ensemble and retain the original state with the probability $\tilde{q}_{ij}$. The average score S is adjusted in such a way, that the number of lattice states in the ensemble remains constant. After equilibrium is reached, the average score will be

$$S = \exp\left(-\Delta\tau\ E_0\right) \tag{11}$$

and can be used to determine the energy E_0^{proj} of the ground state. Simultaneously, expectation values of other operators can be measured according to (2).

3. APPLICATIONS OF THE PROJECTOR MONTE CARLO METHOD TO THE MASSIVE LATTICE SCHWINGER MODEL

The lattice Hamiltonian of the massive Schwinger model is well known[5]

$$H = \frac{1}{2}\, g^2 a \sum_n (L_n - \alpha)^2 + \frac{1}{2a} \sum_n \left(\chi_n^+\, a_n^+\, \chi_{n+1} + \chi_{n+1}^+\, a_n\, \chi_n\right) + m \sum_n (-1)^n\, \chi_n^+\, \chi_n \tag{12}$$

n runs over the N spatial lattice points. The fermion creation and destruction operators χ_n^+ and χ_n sit on the lattice points, the gauge boson creation and destruction operators a_n^+ and a_n sit on the links between the lattice points n and $n+1$, L_n is the boson occupation number operator, g^2 is the coupling constant, the θ-angle, $\theta = 2\pi\alpha$ characterizes the constant electric background field and m is the fermion mass. Equation (12) uses Susskind fermions[20] to prevent fermion doubling.

We represent the Hamiltonian as

$$H = \sum_n h_{n,n+1} \tag{13}$$

$$h_{n,n+1} = \frac{1}{2}\, g^2 a (L_n - \alpha)^2 + \frac{1}{2a}\Big(\chi_n^+ a_n^+ \chi_{n+1} + \chi_{n+1}^+ a_n \chi_n + m(-1)^n \chi_n^+ \chi_n\Big) \ .$$

Both parts of the Hamiltonian

$$H_1 = \sum_{n_{\rm odd}} h_{n,n+1} \quad ; \quad H_2 = \sum_{n_{\rm even}} h_{n,n+1} \tag{14}$$

are sums of commuting operators. We introduce lattice eigenstates at times t_j in the occupation number representation

$$|t_j\rangle = \prod_n \ (\chi_n^+)^{i_{j,n}} \ (a_n^+)^{k_{j,n}} \ |0\rangle \tag{15}$$

where $i_{i,n}$ $(= 0, 1)$ and $k_{i,n}$ (= integer) are the fermion and boson occupation numbers.

The matrix elements of the operators U_i between the eigenstates $|i_{j,n}, i_{j,n+1}, k_{j,n}\rangle$ are well known.[5] Only few elements are different from zero

$$\begin{aligned}
U_i\,|1,1,\ell\rangle &= A_1\,|1,1,\ell\rangle \\
U_i\,|0,0,\ell\rangle &= A_2\,|0,0,\ell\rangle \\
U_i\,|1,0,\ell\rangle &= a_1\,|1,0,\ell\rangle - a_2\,|0,1,\ell-1\rangle \\
U_i\,|0,1,\ell\rangle &= a_3\,|0,1,\ell\rangle - a_4\,|1,0,\ell+1\rangle
\end{aligned} \tag{16}$$

The A_i and a_i are given in Ref. 5. In Table I we give our splitting of the matrix elements into the probabilities P_{ij} and scores S_{ij}.

We calculate also the expectation values of the Hamiltonian H. Our starting states $|\phi\rangle$ are a half-filled fermion band

$$|\phi\rangle = \frac{1}{\sqrt{2}} \left[|1,0,1,0,\ldots\rangle + |0,1,0,1,\ldots\rangle \right]$$

and a boson state with all occupation numbers $k_{i,n} = 0$.

There arises one problem applying the ensemble projector method to a fermion model like the Schwinger model, where matrix elements and scores of both signs are present, see Table I. In fact the sign of the total score of a state will change stochastically during the updating of the state. Only the total score is of importance, therefore no problems would arise if, at the end of the calculation, we reject all states with negative total scores. In this case, it is justified to use for the replication the nonnegative values of the individual scores. A subset of these states with positive total score are the states which are periodic in time direction. These were the only states used formerly in the local Hamiltonian Monte Carlo method.[3–5] In fact using only the states with positive total score we use about half of all possible states and therefore more than in the former method. Using half of all states should be sufficient to calculate the expectation values. In fact, since the sign of each state changes stochastically during the updating, we could as well use only the states with total score of negative sign. In fact we do both, calculating the expectation values of matrix elements separately for the two ensembles of states with total score of positive and negative sign. We expect, that both expectation values should agree. Furthermore, if we calculate the expectation value of the Hamiltonian, both values should agree with the ground state energy determined from the average score according to (11). We will see in the next section, that this is really the case in our Monte Carlo

calculation. Therefore we are confident, to apply the ensemble projector Monte Carlo method also to models with more than one spatial dimension where only the subset of states periodic in temporal direction, which could be used in the local Hamiltonian method, would not be representative for the model.

4. RESULTS AND DISCUSSION

In order to demonstrate the problems of the simple projector Monte Carlo method, without the replication step, we present in Fig. 1 a distribution of total scores obtained for the Schwinger model using this method. The score fluctuations increase dramatically with the lattice size, in the example of Fig. 1 we use $N_x = 20$ spatial lattice positions and $2L = 40$ time slices. The relative weights of the lattice configurations in this example differs by 3-4 decades. Only about 10^{-3} of all configuration sampled in the Monte Carlo calculation contribute significantly to the expectation values calculated, this leads to large fluctuation in the results.

In our ensemble projector Monte Carlo calculation we use again $N_x = 20$ spatial lattice positions and ensembles of about 500-2000 lattice states. The $\Delta\tau$ steps have a value of $\Delta\tau = 0.1$, in units of the spatial lattice spacing $a = 1$. All our calculations reported here are for a vanishing background field $\alpha = 0$. Our calculations are for two values of the gauge coupling constant $g = 0.2$ and $g = 0.57$. In Fig. 2 we plot for two different sets of parameters the expectation values for E_0^+, E_0^- and $E_0^{\rm proj}$ obtained from our ensemble of states always after 10 iteration steps $\Delta\tau$ in time direction. The measurements start after an initial set of 300 iteration steps. As can be seen, after a total of about 300 iteration steps, the ensemble of states seems to have attained thermal equilibrium. The

numbers of states with positive and negative total scores fluctuate during the updating but agree usually to some 5% or better.

In Table II and Figs. 3 and 4 we present our results, the ground state energies per lattice point, for two values of the gauge coupling constant g and different values of the fermion mass m. The three separate expectation values $\langle E_0^+ \rangle$, $\langle E_0^- \rangle$ and $\langle E_0^{\rm proj} \rangle$ obtained with the ensemble projector method are compared with each other and with the result of the local Hamiltonian Monte Carlo method using the method and computer program described in Ref. 5. We find all four expectation values to agree within the statistical errors.

Per point calculated we use with each of the two methods around 4-5 minutes of IBM 3081 time. The statistical errors of the ensemble projector Monte Carlo method, after a sufficient number of heating interactions, seem to be not larger than the errors of the local Hamiltonian Monte Carlo method.

ACKNOWLEDGEMENTS

One of the authors (J.R.) would like to thank Prof. S. D. Drell for the possibility to stay in the SLAC – Theory Group, where the paper was completed. He furthermore acknowledges discussions with R. Blankenbecler. This work was supported by the Department of Energy under contract DE-AC03-76SF00515.

REFERENCES

1. K. G. Wilson, Phys. Rev. D 10, 2445 (1974); M. Creutz, Phys. Rev. Lett. 45, 313 (1980); Phys. Rev. D 21, 2308 (1980).
2. J. Kogut and L. Susskind, Phys. Rev. D 11, 395 (1975).
3. J. E. Hirsch, R. L. Sugar, D. J. Scalapino and R. Blankenbecler, Phys. Rev. B26, 5033 (1982).
4. D. Martin and S. Otto, Nucl. Phys. B203, 193 (1982).
5. J. Ranft and S. Schiller, Phys. Lett. 122B, 403 (1983); A. Schiller and J. Ranft, Nucl. Phys. B225 [FS 9], 204 (1983); J. Ranft, Phys. Lett. 133B, 423 (1983).
6. J. Ranft and A. Schiller, Phys. Lett. 140B, 239 (1984); J. Ranft and A. Schiller, Nucl. Phys. B251 [FS 13], 764 (1985).
7. J. Ranft and A. Schiller, Phys. Lett. 138B, 166 (1984); A. Schiller and J. Ranft, Leipzig preprint KMU-HEP 84-07 (1984).
8. R. Blankenbecler and R. L. Sugar, Phys. Rev. D 27, 1304 (1983); D. Kung, R. Blankenbecler and R. L. Sugar, preprint SLAC-PUB-3485 (1985).
9. J. Potvin and T. A. DeGrand, Phys. Rev. D 30, 1285 (1984).
10. J. Ranft, Leipzig preprint (1984), to be published in Annalen der Physik (1985).
11. J.-F. Min, J. A. Shapiro and T. A. DeGrand, Rutgers University preprint (1984).
12. D. Dahl and R. Blankenbecler, preprint SLAC-PUB-3484 (1984).
13. S. A. Chin, J. W. Negele and S. E. Koonin, Ann. Phys. 157, 140 (1984).

14. D. K. Campbell, T. A. DeGrand and S. Mazumdar, Phys. Rev. Lett. 52, 1717 (1984).

15. T. A. DeGrand and J. Potvin, Phys. Rev. D 31, 871 (1985).

16. J. Potvin, Colorado University preprint COLO-HEP-88 (1985).

17. M. Hellmund, Leipzig preprint KMU-HEP-85-7 (1985), submitted to Physics Letters.

18. D. Kung, D. Dahl, R. Blankenbecler, R. Deza and J. R. Fulco, preprint SLAC-PUB-3605 (1985), submitted to Phys. Rev. B.

19. A. Schiller and J. Ranft, to be published.

20. L. Susskind, Phys. Rev. D 16, 3031 (1977).

Table I

Probabilities and scores for the massive lattice Schwinger model

Transitions	Probability P_{ij}	Score S_{ij}
$\|1,1,\ell\rangle \rightarrow \|1,1,\ell\rangle$	1	A_1
$\|0,0,\ell\rangle \rightarrow \|0,0,\ell\rangle$	1	A_2
$\|1,0,\ell\rangle \rightarrow \|1,0,\ell\rangle$	$\frac{a_1}{a_1+a_2}$	a_1+a_2
$\|1,0,\ell\rangle \rightarrow \|0,1,\ell-1\rangle$	$\frac{a_2}{a_1+a_2}$	$-(a_1+a_2)$
$\|0,1,\ell\rangle \rightarrow \|0,1,\ell\rangle$	$\frac{a_3}{a_3+a_4}$	a_3+a_4
$\|0,1,\ell\rangle \rightarrow \|1,0,\ell+1\rangle$	$\frac{a_4}{a_3+a_4}$	$-(a_3+a_4)$

Table II

Energy expectation values of the Schwinger model E_0^+, E_0^-, $E_0^{\rm proj}$ calculated using the ensemble projector Monte Carlo method and $E_0^{\rm local}$, obtained from the local Hamiltonian Monte Carlo method.

g	m	E_0^+	E_0^-	$E_0^{\rm proj}$	$E_0^{\rm local}$
0.2	0.	-0.311 ± 0.01	-0.313 ± 0.01	-0.304 ± 0.01	-0.31 ± 0.02
	0.1	-0.318 ± 0.01	-0.318 ± 0.01	-0.310 ± 0.01	-0.29 ± 0.02
	0.2	-0.329 ± 0.01	-0.331 ± 0.01	-0.332 ± 0.01	-0.335 ± 0.02
	0.3	-0.356 ± 0.01	-0.352 ± 0.01	-0.352 ± 0.01	-0.349 ± 0.02
	0.4	-0.392 ± 0.01	-0.392 ± 0.01	-0.388 ± 0.01	-0.382 ± 0.02
	0.5	-0.406 ± 0.01	-0.407 ± 0.01	-0.409 ± 0.01	-0.409 ± 0.02
0.57	0.	-0.271 ± 0.01	-0.277 ± 0.01	-0.265 ± 0.01	-0.26 ± 0.02
	0.1	-0.290 ± 0.01	-0.292 ± 0.01	-0.284 ± 0.01	-0.29 ± 0.02
	0.2	-0.307 ± 0.01	-0.306 ± 0.01	-0.312 ± 0.01	-0.32 ± 0.02
	0.3	-0.341 ± 0.01	-0.345 ± 0.01	-0.343 ± 0.01	-0.34 ± 0.02
	0.4	-0.368 ± 0.01	-0.371 ± 0.01	-0.371 ± 0.01	-0.37 ± 0.02
	0.5	-0.405 ± 0.01	-0.405 ± 0.01	-0.408 ± 0.01	

FIGURE CAPTIONS

Fig. 1. Distribution of the positive total scores for a typical calculation with the projector Monte Carlo method. The lattice states consist of $N = 20$ spatial lattice points and $2L = 40$ time slices.

Fig. 2. Comparison of the ground state energy expectation values E_0^+, E_0^- and $E_0^{\rm proj}$ obtained from our ensemble of states in steps of 10 iterations. The measurements start after an initial set of 300 iterations of the ensemble. (a) $g = 0.2$, $m = 0.3$ and (b) $g = 0.57$, $m = 0.3$.

Fig. 3. Ground state energies per lattice point. The expectation values E_0^+, E_0^- and $E_0^{\rm proj}$ were obtained from about 400 iterations of an ensemble of about 1000 lattice states. The gauge coupling constant is $g = 0.2$. The measured energies are given as function of the fermion mass m.

Fig. 4. As Fig. 3 for a gauge coupling constant $g = 0.57$.

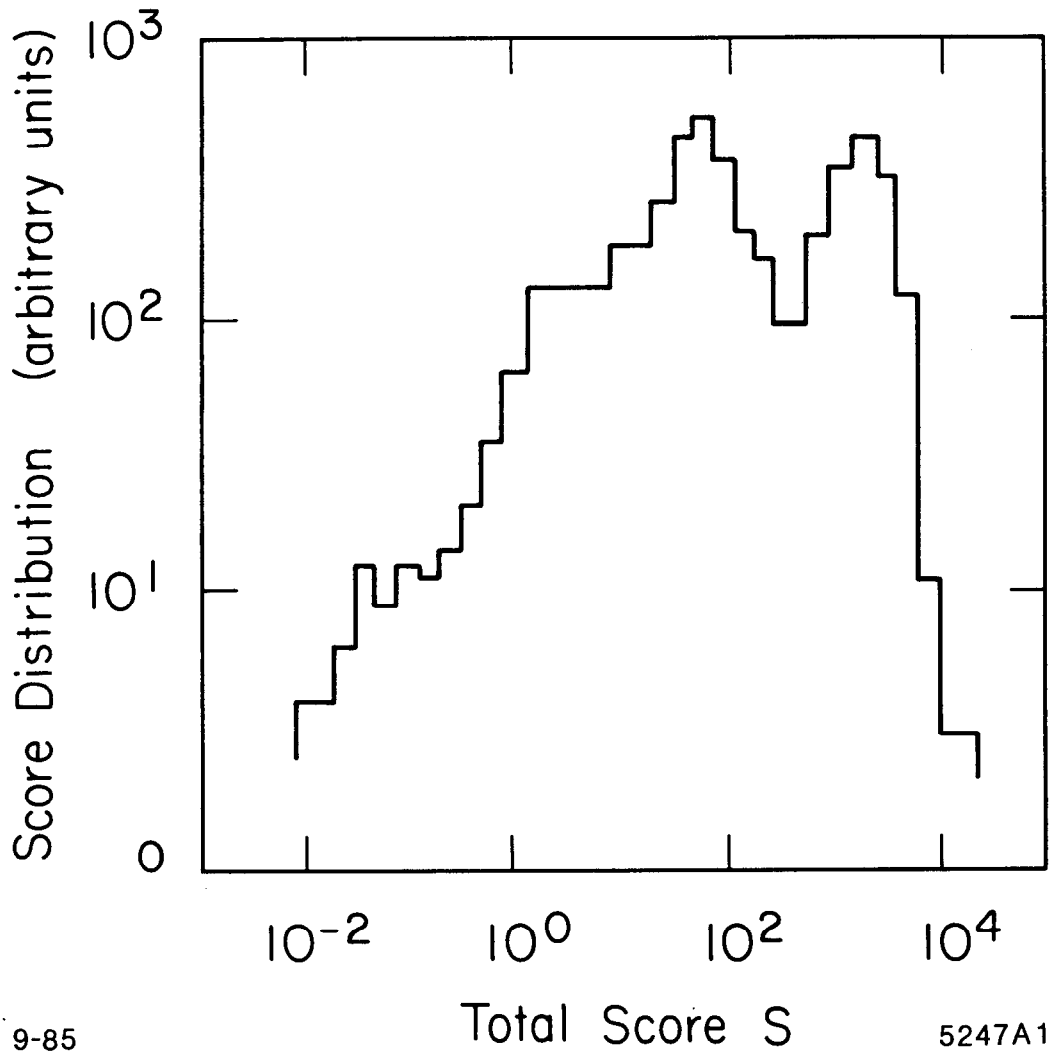
Score Distribution (arbitrary units)
10^3
10^2
10^1
0
10^-2
10^0
10^2
10^4
Total Score S
9-85
5247A1

Fig. 1

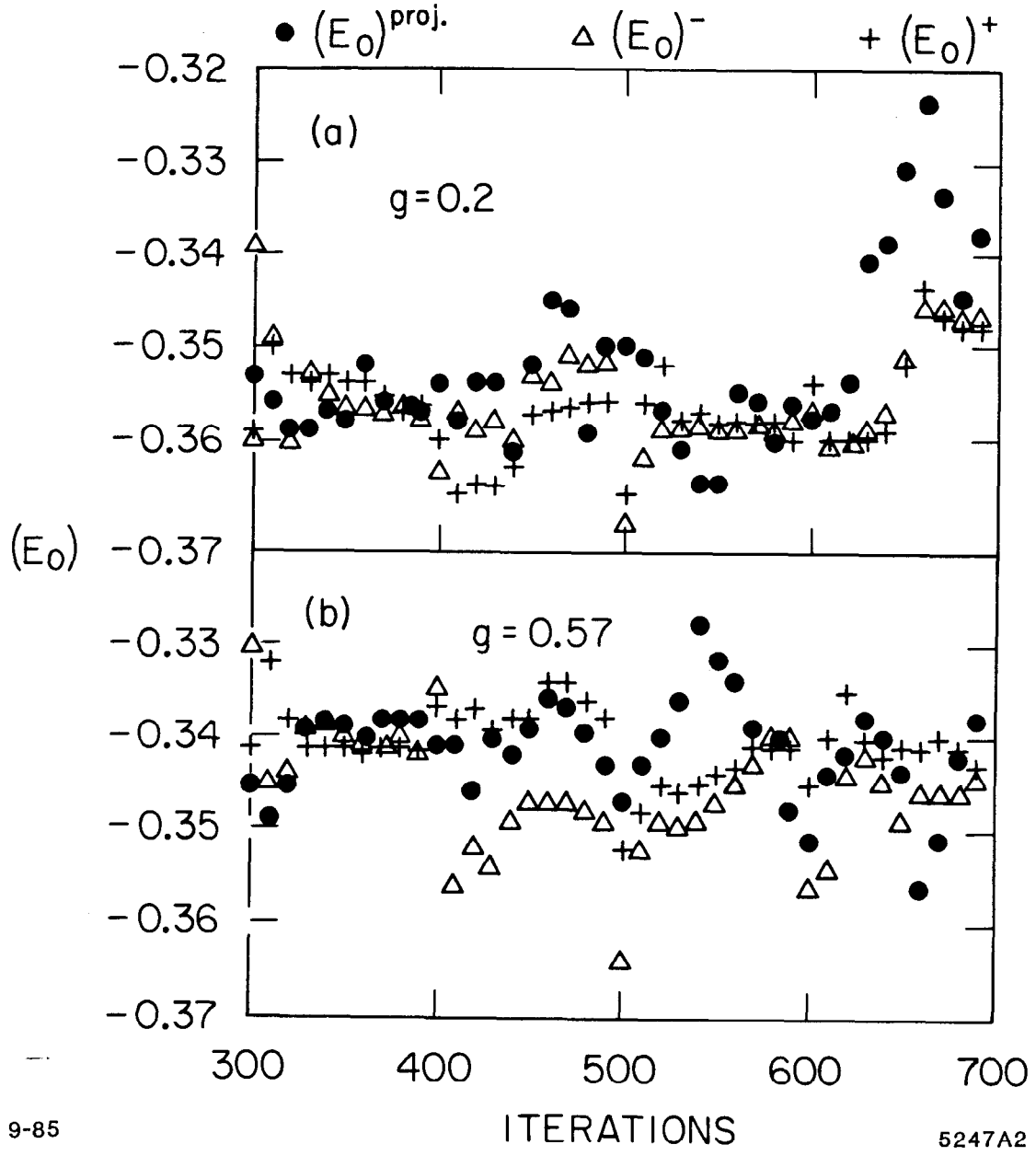
● $(E_0)^{proj.}$
△ $(E_0)^-$
+ $(E_0)^+$
(a)
g=0.2
(b)
g = 0.57
(E_0)
-0.32
-0.33
-0.34
-0.35
-0.36
-0.37
300
400
500
600
700
ITERATIONS
9-85
5247A2

Fig. 2

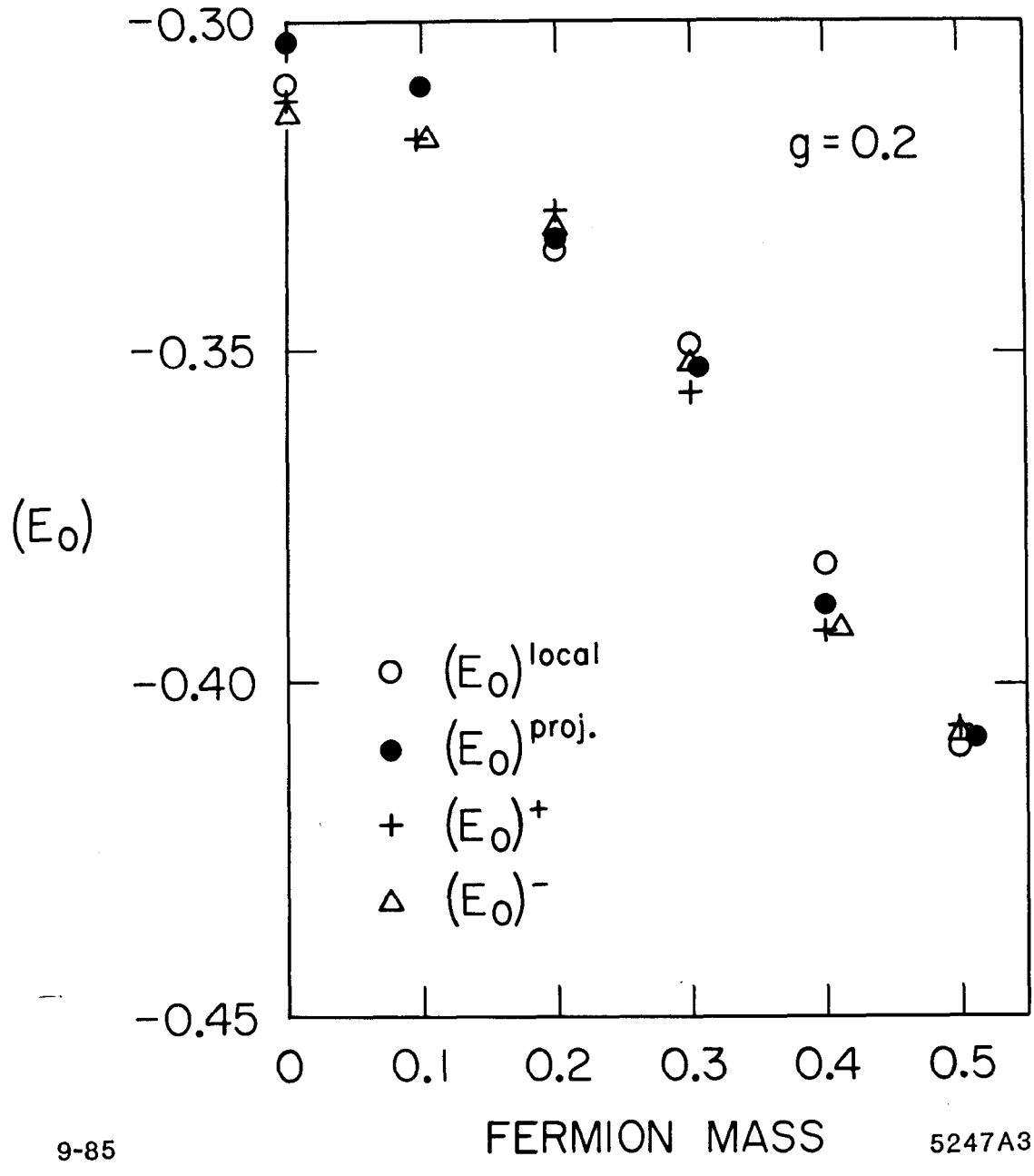
-0.30
-0.35
-0.40
-0.45
(E0)
g = 0.2
(E0)local
(E0)proj.
(E0)+
(E0)-
0
0.1
0.2
0.3
0.4
0.5
FERMION MASS
9-85
5247A3

Fig. 3

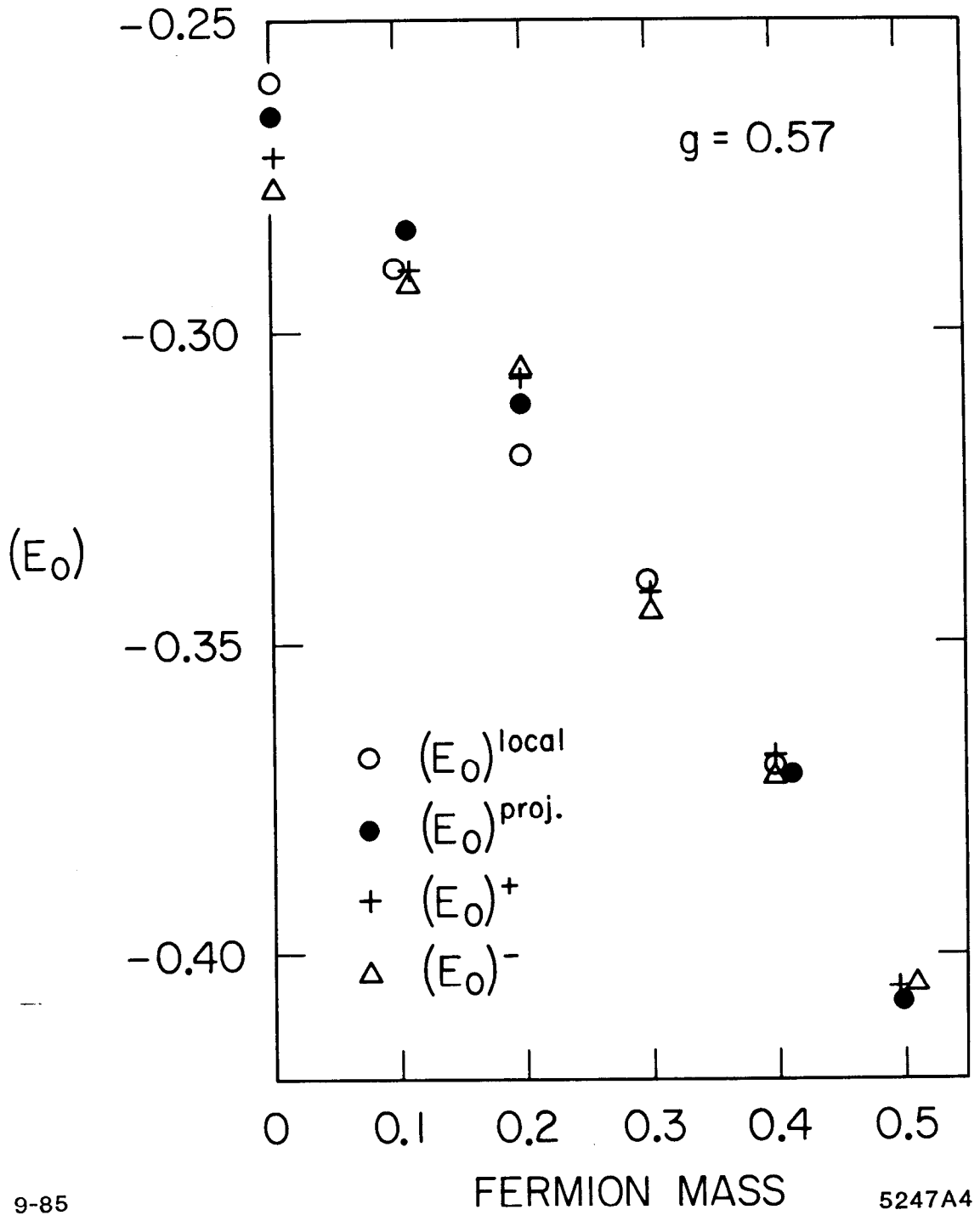
-0.25
-0.30
-0.35
-0.40
(E0)
g = 0.57
(E0)local
(E0)proj.
(E0)+
(E0)-
0
0.1
0.2
0.3
0.4
0.5
FERMION MASS
9-85
5247A4

Fig. 4