# New Proposal for Including Dynamical Fermions in Lattice Gauge Theories: The Compact-QED Case

V. Azcoiti,[a] G. Di Carlo,[b] and A. F. Grillo[b]

*Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain*

(Received 14 June 1990)

We present a new method for including dynamical fermions in lattice gauge theories that can increase the efficiency of Monte Carlo simulations by significantly decreasing the amount of required computer time. The accuracy of the method is demonstrated by comparison with numerical results obtained with other methods in compact QED. New results on the phase transition of QED with massless fermions on $6^4$ and $8^4$ lattices are also presented.

PACS numbers: 11.15.Ha, 02.70.+d, 12.20.Ds

The exact solution of gauge theories with dynamical fermions by means of numerical simulations is a difficult task, owing to the large amount of computer time required to calculate the fermionic determinant, which, in an exact computation, should be evaluated at each link update. Various methods have been proposed for the solution of this problem in the past. Some of them use approximations which introduce systematic errors, and in any case present serious problems of numerical convergence in the physically interesting region of small fermion masses, which in turn introduce new systematic errors associated with necessary extrapolation processes.

In this Letter we present a method for introducing dynamical fermions in lattice computations in which the systematic approximations introduced are well under control. The fundamental advantage of this method consists of the fact that, by determining the effective fermionic action as a function of the plaquette energy, a single fermionic numerical simulation is sufficient to measure the various physical quantities for every value of the coupling constant $\beta$ and for arbitrary number of flavors. Also, the method used for the computation of the fermionic determinant presents the additional feature of allowing the computation of physical quantities for every value of the fermion mass.

In order to test the method, we have compared our results for compact QED in four dimensions with those obtained by Dagotto and Kogut[1,2] using the hybrid algorithm on $6^4$ and $8^4$ lattices, finding perfect agreement. In addition, we have computed the energy per plaquette and specific heat of massless QED around the confining-Coulomb phase transition.

To illustrate how the method works, let us consider compact electrodynamics, regularized on a space-time lattice, written in terms of Kogut-Susskind fermions and of the standard Wilson action for the gauge part:

$$Z=\int [d\bar{\psi}][d\psi][dU]e^{-S_f}e^{-\beta S}$$
$$=\int [dU]\det\Delta(U,m)e^{-\beta S}, \quad (1)$$

where $S_f$ is the Kogut-Susskind fermionic action and $S=\sum_{\rm pl}\mathrm{Re}U_{\rm pl}$ is the pure-gauge Wilson action. $\Delta(m,U)$ in (1) is the lattice Dirac operator, the determinant of which appears when we integrate the fermionic Grassman variables.

The properties of the fermionic matrix $\Delta(m,U)$, together with its gauge invariance, allow us to write[3]

$$\det\Delta(m,U)=m^V+C_1(U)m^{V-2}+C_2(U)m^{V-4}+\cdots$$
$$+C_n(U)m^{V-2n}+\cdots+C_{V/2}(U), \quad (2)$$

where $V$ is the lattice volume.

The coefficients $C_n(U)$, which depend on the gauge configuration $\{U\}$, get contributions from the products of all possible closed loops of total perimeter $2n$ which do not touch. In particular, $C_1$ is constant and $C_2$ is proportional to the average plaquette energy, apart from a constant.

With this in mind we can write

$$\det\Delta(m,U)=\det\Delta(m,S(U),S_i(U)), \quad (3)$$

where $S(U)$ is the pure gauge action and $S_i(U)$ is the collection of all other gauge-invariant operators necessary to build up the coefficients $C_n(U)$ with $n>2$. Using relation (3) the partition function can be rewritten as

$$Z=\int [dU]\delta(S(U)-E)\left[\prod_i \delta(S_i(U)-E_i)\right]e^{\beta E}$$
$$\times\det\Delta(m,E,E_i)dE\prod_i dE_i$$
$$=\int\left[\prod_i dE_i\right]dE\,N(E,E_i)e^{\beta E}\det\Delta(m,E,E_i), \quad (4)$$

with

$$N(E,E_i)=\int [dU]\delta(S(U)-E)\prod_i \delta(S_i(U)-E_i)$$

the density of states of fixed "energies" $E,E_i$. Defining then the average value of the fermionic determinant at fixed energy $E$ as

$$\overline{\det}\Delta(E,m)=\frac{\int(\prod_i dE_i)N(E,E_i)\det\Delta(m,E,E_i)}{\int(\prod_i dE_i)N(E,E_i)}, \quad (5)$$

one gets, for the partition function,

$$Z=\int dE\, N(E)e^{\beta E}\overline{\det}\Delta(E,m)=\int [dU]e^{-S_{\rm eff}}, \quad (6)$$

where $N(E)$ is the density of states at energy $E$,

$$N(E)=\int \left[\prod_i dE_i\right] N(E,E_i)$$

$$=\int [dU]\delta(S(U)-E). \quad (7)$$

Equations (6) and (7) define an effective action

$$S_{\rm eff}=\beta S(U)-\ln\overline{\det}\Delta(m,S(U)). \quad (8)$$

The method we propose consists in first determining $\ln\overline{\det}\Delta(m,E)$ numerically, as a function of the energy $E$, and afterwards in performing a numerical simulation of the equivalent pure gauge model (8) to measure the thermodynamical quantities. The first step then consists in the generation of gauge configurations at fixed energy $E$ with a microcanonical process and in the determination of the average fermionic determinant over the different configurations generated. By repeating the procedure for different values of $E$ one finally gets an expression for $\ln\overline{\det}\Delta(m,E)$ by means of an interpolation of the points obtained.

Since the numerical determination of expression (5) is the crucial step of our method, some discussion about the feasibility of this computation is in order. The nonlocal character of the fermionic determinant implies that, computing the fermionic determinant on configurations generated with the pure gauge probability distribution at a fixed $\beta$, one has large fluctuations that make its determination very difficult. On the other hand, by fixing the energy of the configurations over which the determinant is computed, a large part of the fluctuations disappear. This can be explained by considering that the coefficients of Eq. (2) contain products of the plaquette energy with, in general, large coefficients; moreover, fixing the energy prevents the system, near the phase transition, from fluctuating between different vacua, so reducing the fluctuations of larger loops. The remaining fluctuations are associated with transformations which leave the average energy per plaquette (but not more complicated loops) constant. In these circumstances the important quantity to inquire about is the amount of computer time needed to measure $\ln\overline{\det}\Delta(m,E)$ with the precision necessary for the method to lead to reasonable results. The answer to this question is in general far from trivial; however, a simple analysis of the feasibility of the method can be carried out under some general assumptions.

Figure 1 shows the histogram of the logarithm of the fermionic determinant at $m=0.1$ and $E/6V=0.5103$ for a $4^4$ lattice. As can be seen, the histogram can be very well approximated by a Gaussian (continuous line). Based on this result, let us consider a toy model in which the probability distribution $P_E(x)$ of the logarithm of the fermionic determinant at energy $E$ is described by a

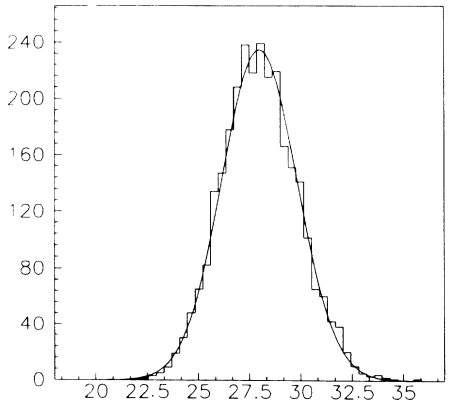


FIG. 1. Probability distribution of the logarithm of the fermionic determinant at fixed energy on a $4^4$ lattice; a Gaussian distribution is superimposed (continuous line).

Gaussian function,

$$P_E(x)=Ce^{-\alpha(x-x_0)^2}, \quad (9)$$

where $C$ is a normalization constant and $\alpha$ and $x_0$ are parameters which depend on the volume $V$, the energy $E$, and mass $m$. From the above distribution one can obtain through an elementary calculation

$$\ln\overline{\det}\Delta(m,E)=x_0+1/4\alpha. \quad (10)$$

Since $x_0$ is essentially the average value of the logarithm of the determinant at energy $E$, $x_0=\overline{\ln\det}\Delta(m,E)$, it will in general be a linear function of the volume $V$, thus giving a contribution to the effective action (8) of the same order as the pure gauge term. The crucial point is the dependence of $\alpha$, i.e., of the width of the Gaussian (9), on $V$. Let us assume that $\alpha\to 0$ as $V^{-\nu}$ when $V\to\infty$. We can have three cases. (i) $\nu>1$: $1/4\alpha$ diverges as $V^{\nu}$ and in the thermodynamical limit will be the dominant contribution to the effective action (8). (ii) $\nu=1$: $1/4\alpha$ is comparable to $x_0$ as well as to the pure gauge term. (iii) $\nu<1$: The contribution of $1/4\alpha$ disappears in the thermodynamical limit.

Case (i) will certainly be surprising, since it will imply that, in the thermodynamical limit, the physical results do not depend on the coupling constant. Case (ii) is the most probable from a statistical point of view, but even (iii) is not absurd, since it implies that the fluctuations of the logarithm of the determinant are damped as a consequence of the fixing of the energy of the configurations.

In Fig. 2 we show the behavior of the fluctuations of the logarithm of the fermionic determinant at $m=0.1$ as a function of $E/6V$ on $4^4$, $6^4$, and $8^4$ lattices. The weak dependence of the fluctuations on the volume which one observes in the figure (analogous results can be obtained even at $m=0$) seem to favor the behavior described in (iii); in which case the contribution of $1/4\alpha$ to the effective action is a pure volume effect, in the sense that

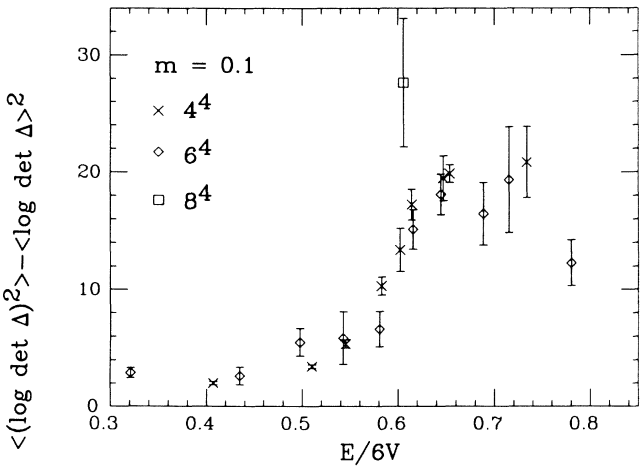


FIG. 2. Fluctuations of the logarithm of the fermionic determinant at fixed energy as a function of the normalized energy, on $4^4$, $6^4$, and $8^4$ lattices.

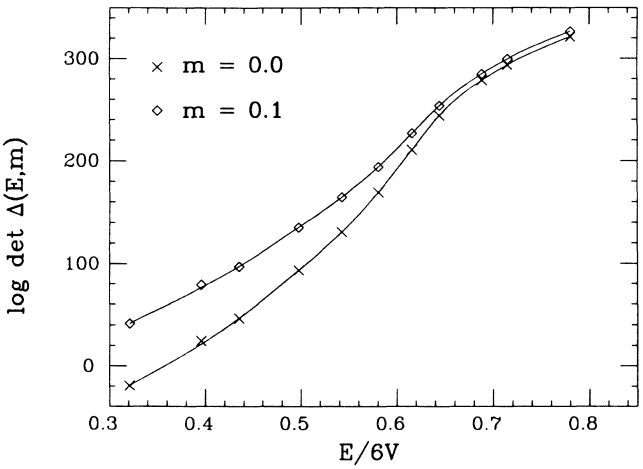


FIG. 3. Numerical results for the effective fermionic action on a $6^4$ lattice, vs the normalized plaquette energy at $m=0.1$ and 0.0. Statistical errors are not larger than the points.

it will disappear in the large-volume limit. This result allows the justification of the feasibility of the numerical computation of $\ln\overline{\det}\Delta(m,E)$.

The interpretation of the results shown in Fig. 2 in the light of our toy model, though not providing a rigorous proof, suggests that the method proposed can be applied, with a reasonable amount of computer time, to realistic models and larger lattices.

We will now briefly describe the details of our simulations and some of the results obtained. A more detailed analysis will appear in a forthcoming paper.[4]

Standard over-relaxation[5] has been used for the microcanonical process to generate fixed-energy gauge configurations. On the $4^4$, $6^4$, and $8^4$ lattices, 100, 500, and 1000 over-relaxation iterations separate successive gauge configurations on which one measures the fermionic determinant. In the computation of the fermionic determinant we have used a standard library diagonalization routine as well as a modified Lanczos algorithm; in both cases it is possible to compute all the eigenvalues of the zero-mass fermionic matrix, from which one can reconstruct the determinant at every mass.

Figure 3 shows the numerical results obtained for $\ln\overline{\det}\Delta(m,E)$ on a $6^4$ lattice as a function of the normalized plaquette energy at typical values of the fermion mass ($m=0.1,0.0$). In this calculation, we have used 100–500 measurements per point and the statistical errors have been computed by the jackknife method. Interpolating the plotted points with a polynomial (solid lines in the figure) one obtains the corresponding expression for the effective fermionic action, which now can be used to perform a standard simulation with action (8).

Figure 4 shows the results obtained for the plaquette energy versus $\beta$ on a $6^4$ lattice and at fermion masses 0.1,0.0. Our results at $m=0.1$ are in excellent agreement with those of Dagotto and Kogut.[1]

An analysis of the specific heat analogous to the one developed in Ref. 6 places the critical couplings at ($\beta=0.8854(3)$, $m=0.1$) and ($\beta=0.8540(5)$, $m=0.0$). From the same analysis we get for the height $h_c$ of the peak of the specific heat the value $h_c=8.9(2)$ at $m=0.1$ and $h_c=8.2(3)$ at $m=0$, against the value $h_c=7.57(13)$ at $m=\infty$ (quenched case). These results tell us that light fermions induced a faster change in the mean energy per plaquette around the phase transition point, again in good agreement with Ref. 1.

We have also performed simulations on $8^4$ lattices using few measurements per point when computing the effective fermionic action (8). This calculation can be meaningful if, as suggested by Fig. 2, the fluctuations of the logarithm of the fermionic determinant at fixed energy are weakly dependent on the lattice volume. Proceed-

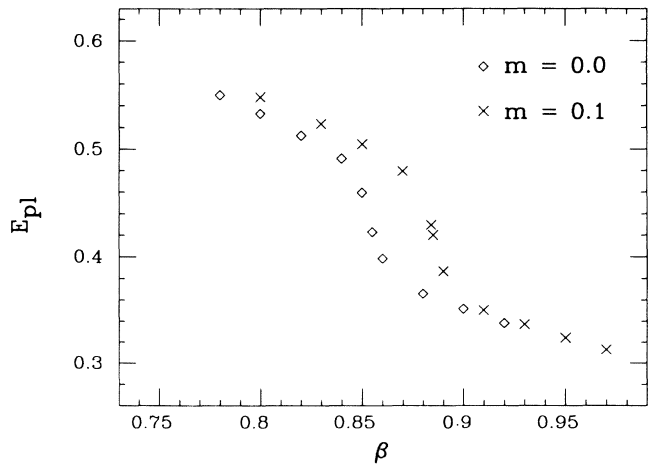


FIG. 4. Numerical results for the mean plaquette energy vs $\beta$ on a $6^4$ lattice at $m=0.1$ and 0.0. Statistical errors are not larger than the points.

ing in the same way as in the $6^4$ case, we have found for the $8^4$ lattices very long metastability signals at ($\beta=0.894$, $m=0.1$) and ($\beta=0.869$, $m=0$). In the $m=0.1$ case, the two coexistent states were located at $1.0-\mathrm{Re}U_{\mathrm{pl}}=0.380,0.450$ (again in good agreement with results reported in Ref. 2), whereas for massless fermions the two states were located at $1.0-\mathrm{Re}U_{\mathrm{pl}}=0.375,0.465$. These results imply a gap for the energy $\Delta E=0.07$ at $m=0.1$ and $\Delta E=0.09$ at $m=0.0$, against the value $\Delta E=0.045$ at $m=\infty$.[6] The effect of light fermions on the phase transition is again manifested by an important increasing of the latent heat. Results on the specific heat as well as a precise determination of the critical couplings for the $8^4$ lattice can be found in Ref. 4.

The errors reported in the figures are purely statistical, associated with the pure gauge simulation with the effective action (8). To estimate the systematic errors connected with the procedure applied in the determination of the effective fermionic action, we have performed simulations using different interpolation functions as well as using curves similar to those plotted in Fig. 3 obtained by grouping the measurements at each point in independent samples. The results obtained in this way for the mean energy per plaquette and specific heat were always compatible, suggesting that systematic errors are less than the statistical ones.

The principal advantages of this method, compared with other standard ones, consist of the fact that a single fermionic simulation allows the determination of the physical observables as a function of the coupling constant $\beta$ and flavor number $n_f$. Also, the method used for the computation of the fermionic determinant allows us to extract the dependence on the fermionic mass $m$. The method presented in this paper is equally applicable to other gauge groups, as well as to the noncompact formulation of QED and to other regularizations of the Dirac operator on the lattice, such as, for instance, the Wilson fermions.

To better appreciate the usefulness of the method, it has to be considered that the results presented in this Letter have been obtained on a VAX 8650, using less than 800 CPU hours. Results for the chiral condensate versus $\beta$ and for the $n_f=1$ and 16 cases will be reported in Ref. 4.

We thank Dr. A. Vladikas for bringing us his modified Lanczos program. This work has been carried out in the context of a CICYT-INFN collaboration; V. Azcoiti thanks the CICYT institution for financial support.

---

[a]Present address: Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, P.O.B. 13, Frascati, Italy.

[b]Permanent address: Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, P.O.B. 13, Frascati, Italy.

[1]E. Dagotto and J. Kogut, Nucl. Phys. **B295 [FS21]**, 123 (1988).

[2]J. Kogut and E. Dagotto, Phys. Rev. Lett. **59**, 617 (1987).

[3]A. Hasenfratz and P. Hasenfratz, Phys. Lett. **104B**, 489 (1981).

[4]V. Azcoiti *et al.*, INFN report (to be published).

[5]S. L. Adler, Phys. Rev. D **23**, 2901 (1981); M. Creutz, Phys. Rev. D **36**, 515 (1986); F. R. Brown and T. J. Woch, Phys. Rev. Lett. **58**, 2394 (1987); S. L. Adler, Phys. Rev. D **37**, 458 (1989).

[6]V. Azcoiti, G. Di Carlo, and A. F. Grillo, Phys. Lett. B **238**, 355 (1990).