ELSEVIER

5 January 1995

PHYSICS LETTERS B

Physics Letters B 341 (1995) 355–360

The general distribution of Lee-Yang zeros in compact lattice QED

I.M. Barbour [a], R. Burioni [b], G. Salina [c]

[a] *Department of Physics and Astronomy, University of Glasgow, Glasgow G12 8QQ, UK*
[b] *Dipartimento di Fisica, Università di Roma "La Sapienza", INFN Sezione di Roma I, I-00185 Roma, Italy*
[c] *INFN Sezione di Roma II, Dipartimento di Fisica, Università di Roma "Tor Vergata", I-00133 Roma, Italy*

Received 9 September 1994
Editor: R. Gatto

Abstract

In this paper we study the general distribution of the Lee-Yang zeros in the complex mass plane for compact QED. We determine all the zeros of the partition function at strong, intermediate and weak coupling on a 4^4 lattice. Our results give a new picture for the general behaviour of the Lee-Yang zeros for different phases of the system.

1. Introduction

A good understanding of the physical properties of a statistical system and of its thermodynamic behaviour can be obtained by studying the complex zeros of its partition function. The Lee-Yang theorem [1] shows explicitly that knowledge of the distribution of the zeros of the partition function determines the equation of state. In particular, the behaviour of the distribution near the positive real axis (the physical region) is closely related to the phase structure and its nature [2]. This kind of analysis has given interesting results in the study of lattice gauge theories both with and without fermions [3,4]. In these models the partition function can be expanded as a polynomial in two critical parameters, the bare mass ma and the bare gauge coupling constant g, which are supposed to drive two different transitions. In particular, by expressing the partition function as a polynomial in the mass, one obtains an analogous formulation to that of Lee and Yang for magnetic systems.

When one studies lattice gauge theories using numerical simulations, the Lee-Yang theorem works as follows: the (complex) zeros of the partition function which tend toward the real axis as the lattice volume increases give evidence for a phase transition and determine the critical value of the parameter at which it occurs. Moreover, the scaling with the volume of their density and of their distance from the real axis provides information on the genus of the phase transition and on the value of its critical exponents [5,6].

However the numerical determination of the gross shape of the zeros is complicated [4]. In a typical simulation, the degree of the polynomial is of the order of the number of lattice sites N, which can be large, varying from 4^4 to 10^4 for this kind of simulation [4,8]. Moreover, the coefficients vary in magnitude over a huge range and are only measured to some precision. Hence the determination of the zeros can be affected by these uncertainties and by the systematic and rounding errors due to the particular algorithm used for the root finder.

In this paper we study in detail the general distribution of the Lee-Yang zeros for compact QED on a 4^4 lattice at three different values of the coupling constant, $\beta = 0.0$, $\beta = 1.5$ and $\beta = 0.885$. At $\beta = 0$ the

Elsevier Science B.V.
SSDI 0370-2693(94)01323-3

system is in a confined phase for all m and at $\beta = 1.5$ it is in a Coulomb phase for all m. At the intermediate coupling, $\beta = 0.885$, there is a critical value of the mass, m_c, at which the system appears to signal an infinite volume phase transition.

The zeros are found using the mass shift method [8] together with a new algorithm for finding the roots of the polynomial. This new algorithm avoids the rounding errors introduced by deflation of the polynomial.

Using this method we are able to determine with very good accuracy the complete set of roots for the partition function at strong, weak and intermediate coupling. The value of the critical mass agrees with previous results [8]. However the general shape of the zeros obtained with the new method presents a characteristic pattern which agrees with rigorous theorems [13] in the strong coupling region but gives an unexpected behavior at intermediate and weak coupling.

The paper is organized as follows:

In Section 2 we review the expansion of the partition function for compact U(1) as a polynomial in the fermion mass.

In Section 3 we discuss the mass shift method used in [8] and introduce the new algorithm for finding the zeros of the polynomial. This algorithm (the contour method) is based on standard Cauchy theorems of integration in the complex plane.

In Section 4 we discuss the results obtained for the general distribution of the zeros on a 4^4 lattice.

We emphasize that our results on the 4^4 lattice give only the general distribution of the zeros for different phases of the system. The detailed nature of these phases and the critical indices can only be determinate on much larger lattices. The procedures described below can be extended to such lattices ([14,15]).

2. The partition function of compact U(1) as a polynomial in the fermion mass

We regularise our theory on the lattice by using the Wilson action $S_G[\{U\},\beta]$ for the compact gauge fields and the Kogut-Susskind action $S_F[\{U\},m]$ for the fermions. In this formulation we have four flavours degenerate in mass. Integration over the Grassmann fermionic fields gives the determinant $\det M[\{U\},m]$, where M is the fermion matrix. By introducing the updating fermion mass, m_0, (see [8]) and recalling the irrelevance of overall multiplicative factors in the partition function, we define the partition function as:

$$Z[m,\beta] = \frac{\int[dU]\,\det(M[m])e^{-S_g[\beta]}}{\int[dU]\,\det(M[m_0])e^{-S_g[\beta]}} = \frac{\int[dU]\,\frac{\det(M[m])}{\det(M[m_0])}\det(M[m_0])e^{-S_g[\beta]}}{\int[dU]\,\det(M[m_0])e^{-S_g[\beta]}} = \left\langle \frac{\det(M[m])}{\det(M[m_0])} \right\rangle_{P[m_0,\beta]}. \quad (1)$$

This just states that the partition function is the vacuum expectation value of the determinant ratio $\det M[m]/\det M[m_0]$. This ratio is a polynomial in m^2 proportional to the characteristic polynomial of $M[m=0]$. Its coefficients are measured over an ensemble of configurations generated by hybrid Monte Carlo simulation, using the probability weight

$$P[\{U\},m_0,\beta] = \frac{\det M[\{U\},m_0]e^{-S_G[\{U\},\beta]}}{\int[dU']\det M[\{U'\},m_0]e^{-S_G[\{U'\},\beta]}}. \quad (2)$$

On each configuration of the ensemble, the Lanczos algorithm, without reorthogonalisation, is used to find all the eigenvalues of the massless fermion matrix $M[m=0]$. From these eigenvalues the coefficients of the polynomial and $\det(M[m_0])$ can be easily generated. For details, the reader is referred to [8].

By tuning $m_0 a$ to be near the critical mass $m_c a$ we enforce the weight of Eq. (2) to overlap strongly with the distribution of the observable $\det M[m]/\det M[m_0]$. Thus, we can obtain numerically reliable results for m close to m_0.

3. The determination of the zeros

The determination of the gross shape of the zeros is non-trivial. On a lattice with N sites, the partition function is a polynomial of order $N/2$ in m^2, and the range of the coefficients is large [8]. With this kind of data, standard root finders suffer from several problems [4]. One of the most important is that unless the starting point is very near a complex zero, the root finder is not expected to converge. This problem is enhanced when one has to face huge variation in the values of the coefficients of the polynomials. Moreover, once one finds the zero, the usual deflation algorithm lowers the precision at each step. After several deflations the results become unreliable.

On the other hand one also has to consider that systematic and statistical errors in the coefficients may alter the shape of the zeros [7].

In [8] a method for finding the complex zeros of $Z[m,\beta]$ was presented, based on a standard root finding algorithm developed by Muller and on a second arbitrary mass parameter $\widehat{m}$, the "mass shift". This parameter was introduced in order to solve some of the problems previously cited.

We briefly recall how the "mass-shift" method works. Using the properties of the Kogut-Susskind fermion matrix for a finite lattice of size N we can express $\det M[m]$ as a polynomial in $(m^2 - \widehat{m}^2)$; essentially it is a Taylor expansion around $\widehat{m}$. Therefore, the ratio of interest $\det(M[m])/\det(M[m_0])$ is written as

$$\frac{\det(M[m])}{\det(M[m_0])} = \sum_{n=0}^{N/2} e^{x_n} \frac{(m^2 - \widehat{m}^2)^n}{\det(M[m_0])} = \sum_{n=0}^{N/2} e^{c_n} (m^2 - \widehat{m}^2)^n \tag{3}$$

where

$$c_n \equiv x_n - \ln \det M[m_0] \; . \tag{4}$$

The partition function becomes a finite polynomial in m:

$$Z[m,\beta] = \sum_{n=0}^{N/2} \langle e^{c_n} \rangle_{P[m_0,\beta]} (m^2 - \widehat{m}^2)^n = \sum_{n=0}^{N/2} e^{\overline{C}_n} (m^2 - \widehat{m}^2)^n \tag{5}$$

where the logarithm of the averaged coefficients $\overline{C}_n$ is defined through the equation:

$$e^{\overline{C}_n} \equiv \langle e^{c_n} \rangle_{P[m_0,\beta]} \; . \tag{6}$$

The parameter $\widehat{m}$ is a shift that does not alter the zeros of the partition function. The mass-shift method attempts to solve the problems previously cited in the following way. We used the root finder based on Muller's algorithm on each of the polynomials arising from different choices of $\widehat{m}$ to evaluate the zeros in m near $\widehat{m}$. The same zeros should appear for adjacent choices of $\widehat{m}$ if they are true zeros of the polynomials. Indeed $\widehat{m}$ works as a starting point for a Taylor expansion of the partition function in $(m^2 - \widehat{m}^2)$: if $(m^2 - \widehat{m}^2)$ is small enough the last terms in the polynomial give negligible contributions. For a given $\widehat{m}$ it is not possible to determine accurately all the zeros of the partition function but only those which are in the neighbourhood of $\widehat{m}$.

In [8] we used several real and imaginary values of $\widehat{m}$. Then the coefficients of the polynomial are real. In order to study the whole distribution of the zeros one needs to introduce complex values of $\widehat{m}$. This means that the coefficients can be complex. Therefore we need a root finding algorithm which can efficiently handle a polynomial with complex coefficients and which avoids the errors associated with deflation. We briefly outline the main steps of this method.

Suppose that $F(z)$ is a differentiable function [1] in a domain R containing a simple loop L and all points inside L. Then if $F(z)$ has no poles or zeros on L:

$$\frac{1}{2i\pi} \int_L dz \frac{F'(z)}{F(z)} = N - P \tag{7}$$

where N is the number of zeros of the function $F(z)$ in the region R and P is the number of poles, each counted according to its multiplicity.

Eq. (7) can be used to determine the number of zeros of $F(z)$ present in the region R since $P = 0$ for a polynomial. Then the numerical value of each zero is found by minimizing $|F(z)|$ in R. The vanishing of $|F(z)|$ at the minimum is cross-checked by calculating the integral on a little circle around the point returned by the minimization. If the integral is equal to unity a standard method (for example Laguerre) polishes the numerical value of the zero and increases its precision.

In particular, we divide the complex plane into regions of a given size and calculate the number of the zeros in each region. For each region, starting from a random point we minimize the function $|F(z)|$ storing the path history to avoid superposition. When a minimum is reached, we verify and polish it. The pro-

[1] In our case $F(z)$ is the partition function, Z, considered as an analytic function of m^2.

cedure is iterated till all the zeros inside each region are found.

Clearly this procedure is not affected by the problems caused by deflation and slow convergence. It still suffers, though, from the fact that, as one looks for zeros further and further away from a given $\widehat{m}$, more and more coefficients of the polynomial control the position of the zero. Thus the value of Z will be sensible upon delicate cancellations among higher and higher powers in the polynomial expansion (5). In this way spurious zeros may appear. Only the zeros that reproduced themselves as $\widehat{m}^2$ is varied are taken as genuine zeros of the partition function.

There are flaws in the results presented in Ref. [10] arising from the above effect which we discuss at the end of Section 4. We present the corrected results below.

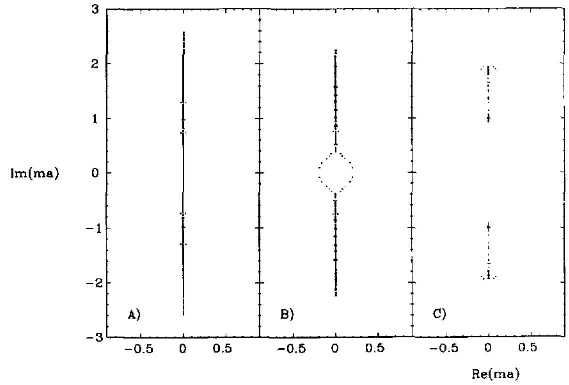

Fig. 1. Complex zeros for a 4^4 lattice at three different β values. A) The 256 complex zeros at $\beta = 0.0$. B) The 256 complex zeros at $\beta = 0.885$. C) Some of the complex zeros at $\beta = 1.5$.

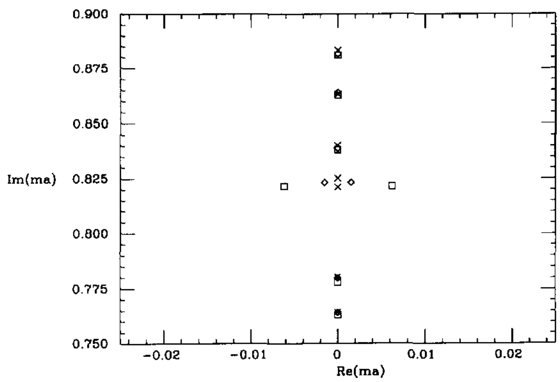

Fig. 2. Behaviour of a given complex zero at $\beta = 0.0$ for different numbers of measurements. The results are superimposed: squares for the zeros obtained after 300 measurements, diamonds after 350 measurements and crosses after 400 measurements.

4. The gross shape of the Lee-Yang zeros

Simulations were performed on a 4^4 lattice at $\beta = 0.0$, $\beta = 0.885$ and $\beta = 1.5$ with periodic boundary conditions for the gauge fields and antiperiodic boundary conditions for the fermion fields. Configurations were generated using the hybrid Monte Carlo algorithm with about 400 iterations to thermalise the system from a cold start. Measurements of the coefficients were made at intervals of $\sim O(1)$ in molecular dynamics time. 400 measurements were made at $\beta = 0.0$ and 300 at $\beta = 0.885$ and $\beta = 1.5$. The evolution of the zeros was monitored every 50 measurements.

Typically we show the zeros obtained from the average over our finite ensemble at each β. However, some indication of their convergence is given by studying their stability as the simulation progressed.

In Fig. 1A we show the 256 zeros of the partition function at $\beta = 0.0$. We used 75 values of $\widehat{m}$ to scan the relevant region of the complex mass plane. Apart from a few zeros with very small real part, they all lie on the imaginary axis. In Fig. 2 we show the behavior of a zero with increasing number of measurements. The real part decreases indicating that the small real parts associated with some zeros are a finite statistics effect.

It is known that at $\beta = 0.0$ the partition function for compact QED is equivalent to the partition function of a monomer-dimer system [11]. In this case the zeros are known to be pure imaginary [12,13]. Our data agree with this analytical result.

In Fig. 1B we show the 256 zeros of the partition function at $\beta = 0.885$ obtained by using 95 different values of $\widehat{m}$ to span the complex plane. Some of the zeros have clearly migrated into the complex plane forming a curve tending to pinch the real m axis. This evidence for a phase transition at $m_c a = 0.194$ is in agreement with the results of [8].

The zeros close to the real axis control any chiral phase transition. They also are given primarily by the coefficients in the polynomial which depend on the longest loops of the gauge fields and thus reflect the non perturbative features of the theory [9,10]. For example the chiral susceptibility is given by:

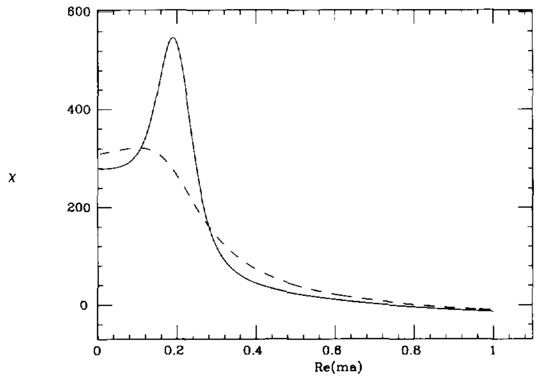

Fig. 3. The chiral susceptibility as a function of ma for $\beta = 0.885$ on a 4^4 lattice: the susceptibility in arbitrary units derived from the whole partition function (solid line) and after the subtraction of the contribution of the zeros closest to the real axis (dashed line).

$$\chi = \partial_{ma} F(ma), \tag{8}$$

where $F(ma)$ is the free energy of the system.

Since the partition function factorizes as:

$$Z(ma) = \prod_i (ma - z_i) \tag{9}$$

where the z_i are its complex zeros, the free energy can be presented as a sum over distinct contributions, each one depending on a different zero:

$$F(ma) = \sum_i \log(ma - z_i) \tag{10}$$

and hence the part responsible for the discontinuity in the susceptibility can be isolated. In Fig. 3 we present a comparison of the chiral susceptibility with and without the contribution of the two symmetric m^2-zeros closest to the real axis at $\beta = 0.885$. It is evident that the divergent part of the chiral susceptibility is associated with these zeros, which are then those possibly leading to the expected phase transition.

The new analysis shows that, apart from this curve of complex zeros cutting the real axis, the other zeros are imaginary. Note, in the region where the zeros tend to be imaginary, those with small real part behave as at strong coupling: with increasing measurements their real part decreases. The curve of zeros around $m = 0$ is stable.

In Fig. 1C we show the zeros of the partition function at $\beta = 1.5$ obtained using 30 different values of $\widehat{m}$. Not all zeros were found because of their high density causing effective degeneracies within our numerical accuracy. However no zeros were found with significant real part and our results are consistent with all the zeros at this weak coupling being imaginary with magnitude between 0.93 and 1.92. This scenario does not agree with the one suggested in [8,10], where the root-finder used for the analysis gave evidence of a line of zeros in the complex plane parallel to the real axis. This line is not present anymore in the new analysis and was due to the poor accuracy of the old root-finder. In the free theory with antiperiodic boundary conditions on the fermions, the zeros are purely imaginary and symmetric.

5. Conclusions

In this paper we have presented a careful analysis of the Lee-Yang zeros in the complex mass plane for compact lattice QED on a 4^4 lattice at different gauge couplings.

The behaviour of the distribution of the zeros is found but we can say nothing about their scaling behaviour. Studies are in progress on large lattices to determine the finite size scaling of the zeros close to the real m-axis using the method described above ([14,15]).

Using a dedicated root finder we were able to determine with very good accuracy the whole set of zeros for the partition function of the model. The critical mass found at intermediate coupling $\beta = 0.885$ agrees with that previously obtained. However the general shape of the zeros shows some unexpected and interesting features.

We can distinguish three distinct distributions for the zeros. At strong coupling all the zeros are imaginary (as predicted by [13]) and signal a possible phase transition at $m_c = 0$. As the coupling decreases the zeros close to the real axis migrate into the complex plane and possibly signal a transition at non-zero fermion mass and intermediate coupling. Apart from the critical cut, no zeros were found outside the imaginary axis. This peculiarity can be inferred only by a accurate knowledge of the complete zeros set. At given critical intermediate coupling they presumably retreat into the complex plane and, as the coupling decreases further, they all become imaginary again. Again this situation appears only after an accurate analysis of the distribution of the zeros and was not present in the previous analysis.

Acknowledgements

It is a pleasure to thank L. Cugliandolo, G. Di Carlo, J. Kurchan and A. Vladikas for very useful discussions and suggestions.

References

[1] C.N. Yang and T.D. Lee, Phys. Rev. 87 52404
[2] T.D. Lee and C.N. Yang, Phys. Rev. 87 52410
[3] G. Bhanot et al., Phys. Lett. B 183 (1987) 331; Phys. Lett. B 187 (1987) 381; Phys. Lett. B 188 (1987) 246.
[4] M. Karliner, S.R. Sharpe and Y.F. Chang, Nucl. Phys. B 302 (1988) 204.
[5] R.B. Pearson, Phys. Rev. B 26 (1982) 6285. C. Itzykson, R.B. Pearson and J.B. Zuber, Nucl. Phys. B 220 (1988) 415.
[6] E. Marinari, Nucl. Phys. B 235 [FS11] (1984) 123.
[7] R. Burioni, G. di Carlo and G. Salina, in preparation.
[8] I.M. Barbour, A.J. Bell, M. Bernaschi, G. Salina and A. Vladikas, Nucl. Phys. B 386 (1992) 683.
[9] I.M. Barbour, A.J. Bell and E.G. Klepfish, Nucl. Phys. B 389 (1992) 285.
[10] I.M. Barbour, A.J. Bell, E.G. Klepfish, R. Burioni, A. Vladikas and G. Salina, Nucl. Phys. B 30 Proc. Suppl. (1993) 339.
[11] P. Rossi and U. Wolff, Nucl. Phys. B 248 (1984) 105.
[12] C. Grubrer and H. Kunz, Comm. Math. Phys. 22 (1971) 133.
[13] M. Salmhofer and E. Seiler, Comm. Math. Phys. 139 (1991) 395.
[14] V. Azcoiti, I.M. Barbour, R. Burioni, G. Di Carlo, A.F. Grillo and G. Salina, in preparation.
[15] I.M. Barbour, R. Burioni and G. Salina, in preparation.