THE STEEPEST-DESCENT-METHOD CALCULATION OF GROUND AND EXCITED STATE ENERGIES IN 2 + 1 QED ON A ONE-PLAQUETTE LATTICE

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The steepest descent method is used for the determination of the ground and a few excited states of the compact QED on a lattice with a single plaquette in 2 + 1 dimensions. The results are very easy to obtain and very accurate in both cases of the ground state and the excited ones. The realization of the method we have used in calculated allows to investigate the nonperturbative effects of the theory.

I. INTRODUCTION

In recent papers [1], [2] a new variational method for the determination of the ground and the excited states of a hamiltonian has been proposed. The purpose of this paper is to show how this so-called steepest descent method (SDM) works in the case of the simple U(1) lattice theory with a single plaquette.

The method is based on the use of two evolution equations for the systematic improvements of the variational states.

According to the Ritz variational principle the expectation value of the hamiltonian $\hat{H}$

$$E(\Psi) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{1}$$

reaches its minimum in the true ground state. The gradient of $E(\Psi)$ in the Hilbert space is given by the vector

$$\frac{\delta E(\Psi)}{\delta \langle \Psi |} = \frac{1}{\langle \Psi | \Psi \rangle} \left[\hat{H} - \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right] | \Psi \rangle . \tag{2}$$

In order to reach the minimum of $E(\Psi)$ we have to proceed just in the opposite direction, because this is the direction of the steepest descent of $E(\Psi)$. To

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describe this movement, the evolution parameter τ is introduced. Then the equation describing the motion of the state along the steepest descent of $E(\Psi)$ can be written in the form

$$\frac{\partial|\Psi(\tau)\rangle}{\partial\tau} = -\frac{1}{\langle\Psi|\Psi\rangle}\left[\hat{H} - \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}\right]|\Psi(\tau)\rangle. \tag{3}$$

Eq. (3) conserves the norm of the state vector during the time evolution. Thus for a normalized initial state $\langle\Psi(0)|\Psi(0)\rangle = 1$ it can be simplified to

$$\frac{\partial|\Psi(\tau)\rangle}{\partial\tau} = -[\hat{H} - \langle\Psi|\hat{H}|\Psi\rangle]|\Psi(\tau)\rangle. \tag{4}$$

The evolution according to this steepest descent equation leads to the ground state under the assumption that the initial state has a nonzero overlap with the true ground state.

The equation describing the motion of the state vector to a general stationary state can be obtained in a similar way. The extremalized functional is the variance of the hamiltonian

$$D(\Psi) = \frac{\langle\Psi|\hat{H}^2|\Psi\rangle}{\langle\Psi|\Psi\rangle} - \frac{\langle\Psi\hat{H}|\Psi\rangle^2}{\langle\Psi|\Psi\rangle^2} \tag{5}$$

which is non-negative and vanishes only if $|\Psi\rangle$ is a stationary state of $\hat{H}$. The gradient of this quantity in the Hilbert space is given by

$$\frac{\delta D(\Psi)}{\delta\langle\Psi|} = \left[\frac{\hat{H}^2}{\langle\Psi|\Psi\rangle} - \frac{\langle\Psi|\hat{H}^2|\Psi\rangle}{\langle\Psi|\Psi\rangle^2} - \frac{2\langle\Psi|\hat{H}|\Psi\rangle\hat{H}}{\langle\Psi|\Psi\rangle^2} + \frac{2\langle\Psi|\hat{H}|\Psi\rangle^2}{\langle\Psi|\Psi\rangle^3}\right]|\Psi\rangle. \tag{6}$$

The corresponding steepest descent evolution equation conserves the norm again and for a normalized initial state we have

$$\frac{\partial|\Psi(\tau)\rangle}{\partial\tau} = -[\hat{H}^2 - \langle\Psi|\hat{H}^2|\Psi\rangle - 2\langle\Psi|\hat{H}|\Psi\rangle\hat{H} + 2\langle\Psi|\hat{H}|\Psi\rangle^2]|\Psi(\tau)\rangle. \tag{7}$$

Eq. (7) is convenient for the search of the excited states of the hamiltonian.

One reasonable way of using Eqs. (4), (7) for the systematic improvements of the variational states was proposed in Ref. [1] and was used for the determination of eigenenergies of the anharmonic oscillator. In this paper we follow the same approach and use it for an investigation of the spectrum of the compact QED on a single plaquette in 2 + 1 dimensions. We have obtained eigenergies of the ground and a few excited states for various values of the coupling constant. The results are very satisfactory both for the ground state and the excited ones. This gives us some hope that the method could be useful in more realistic situations.

In Sect. II. we review the formulation of QED in 2 + 1 dimensions on a single plaquette. Sect. III. is devoted to the description of the strategy we have used in the calculations. Our numerical results are discussed there too. The last section contains the conclusions.

II. FORMULATION OF QED IN 2 + 1 DIMENSIONS ON A SINGLE PLAQUETTE

We will use the gauge in which the scalar potential is identically equal to zero.

In two dimensions the vector potential has two components $\boldsymbol{A} = (A_x, A_y)$, which will be the canonical variables. The conjugated momenta are the components of the electric field $\boldsymbol{E} = (E_x, E_y)$ and the hamiltonian of the theory is

$$\hat{H} = \frac{1}{2}\int d^2x (E_x^2 + E_y^2 + B^2) \tag{8}$$

where

$$B = \partial_x A_y - \partial_y A_x \tag{9}$$

is the magnetic field, which has only one component in two dimensions. The canonical equal-time commutation relations have the form

$$[A_i(\boldsymbol{x}), E_j(\boldsymbol{y})] = -i\,\delta_{ij}\,\delta^2(x - y). \tag{10}$$

In the absence of charges the conjugated momenta have to satisfy the Gauss law

$$\partial_x E_x + \partial_y E_y = 0. \tag{11}$$

To give a discrete formulation of this theory on a simple plaquette we shall use here the compact version of QED on a lattice as it is described in Ref. [3]. This version is constructed in correspondence with the lattice formulation of non-Abelian theories.

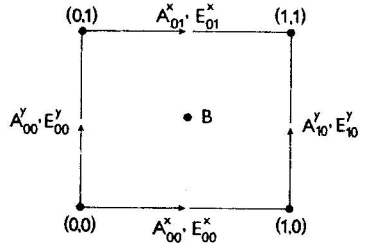

Fig. 1. One plaquette universe.

Our universe will be the lattice which consists of four sites placed in the corners of the square (see Fig. 1.). The spacing of the lattice is a and the

canonically conjugated fields $\boldsymbol{A}$, $\boldsymbol{E}$ are placed on the links of the lattice as shown in Fig. 1. In correspondence with (9) B is defined as the lattice curl

$$B = \frac{1}{a}\,[A^{y}_{10} - A^{y}_{00} - A^{x}_{01} + A^{x}_{00}] \tag{12}$$

and is located at the plaquette centre.

The hamiltonian for the compact QED on a single plaquette has the form [3]

$$\hat{H} = \frac{1}{2}\,a^2\left[(E^{x}_{00})^2 + (E^{y}_{00})^2 + (E^{y}_{10})^2 + (E^{x}_{01})^2 + \frac{2}{g^2 a^4}\,[1 - \cos g a^2 B]\right], \tag{13}$$

where g is the coupling constant. In the $ga^2 \to 0$ limit this hamiltonian corresponds to the continuum case of Eq. (8). The canonical commutators on the plaquette are

$$[A^{a}_{ij},\, E^{b}_{kl}] = -\mathrm{i}a^{-2}\,\delta^{ab}\,\delta^{ik}\,\delta^{jl}. \tag{14}$$

All the variables can be made dimensionless by being divided with the appropriate power of a. If we put a to be equal to unity and canonically rescale

$$\boldsymbol{A} \to \boldsymbol{A}g^{-1} \qquad \boldsymbol{B} \to \boldsymbol{B}g^{-1} \qquad \boldsymbol{E} \to \boldsymbol{E}g, \tag{15}$$

then we can write the final form of the equations we will use:

$$\hat{H} = \frac{g^2}{2}\,[(E^{x}_{00})^2 + (E^{y}_{00})^2 + (E^{x}_{10})^2 + (E^{y}_{01})^2] + \frac{1}{g^2}\,[1 - \cos B] \tag{16}$$

$$B = A^{y}_{10} - A^{y}_{00} - A^{x}_{01} + A^{x}_{00} \tag{17}$$

$$[A^{a}_{ij},\, E^{b}_{kl}] = -\mathrm{i}\,\delta^{ab}\,\delta^{ik}\,\delta^{jl}. \tag{18}$$

The Gauss law implies:

$$\begin{aligned} E^{x}_{00} + E^{y}_{00} &= 0 \qquad & E^{x}_{00} - E^{y}_{10} &= 0 \\ E^{x}_{01} + E^{y}_{10} &= 0 \qquad & E^{x}_{01} - E^{y}_{00} &= 0 \end{aligned} \tag{19}$$

We can satisty the commutation relations (18) by representing the components of the vector potential by the angular variable φ_j and the components of the electric field by the operators $\mathrm{i}\partial/\partial\varphi_j, j = 1, 2, 3, 4$. These operators act on a space quadratically integrable functions with the basis

$$\Psi_{k_1 k_2 k_3 k_4} = \frac{1}{4\pi^2}\,\exp\,[\mathrm{i}\,[k_1\varphi_1 + k_2\varphi_2 + k_3\varphi_3 + k_4\varphi_4]], \tag{20}$$

where $k_j = 0, \pm 1, \pm 2, \ldots$.

If we relate the angular variables to the vector potential components in the following way

$$A^{x}_{00} = \varphi_1 \qquad A^{y}_{10} = \varphi_2 \qquad A^{x}_{01} = \varphi_3 \qquad A^{y}_{00} = \varphi_4, \tag{21}$$

then the Gauss law leads to the conditions

$$k_1 = k_2 = -k_3 = -k_4. \tag{22}$$

Thus in this representation, the eigenstates of our hamiltonian

$$\hat{H} = -\frac{g^2}{2}\sum_{j=1}^{4}\frac{\partial^2}{\partial\varphi_j^2} + \frac{1}{g^2}\,[1 - \cos(\varphi_1 + \varphi_2 - \varphi_3 - \varphi_4)] \tag{23}$$

can be investigated in the subspace with the basis

$$\Psi_K = \frac{1}{4\pi^2}\,\exp\,(\mathrm{i}K\Phi), \tag{24}$$

where $\Phi = \varphi_1 + \varphi_2 - \varphi_3 - \varphi_4$, $\qquad K = 0, \pm 1, \pm 2, \ldots$

III. THE STEEPEST DESCENT DETERMINATION OF THE STATIONARY STATES

The steepest descent Eqs. (4), (7) are rather complicated. They are integro-differential equations with nonlinearities in their integral part. That is why we are not able to solve them exactly. Instead of it we will use some discrete scheme which corresponds to the continuum steepest descent evolution.

The steepest descent equation shows how to do the infinitesimal time steps in the Hilbert space to reach the maximal descrement of the corresponding functional (the mean value of the energy or the mean value of the variance of the energy). To reproduce this in a discrete way we use the following scheme:

We start from some normalized initial state $|\Psi_i\rangle$. As the first step we construct the gradient $|\tilde{\chi}_i\rangle$ of the corresponding functional and normalize it by

$$|\chi_i\rangle = \frac{|\tilde{\chi}_i\rangle}{\langle\tilde{\chi}_i|\tilde{\chi}_i\rangle^{1/2}}, \tag{25}$$

in the second step we construct the state

$$|\Psi_a\rangle = \cos\alpha|\Psi_i\rangle - \sin\alpha|\chi_i\rangle \tag{26}$$

which is normalized automatically, and determine the value of α for which the extremalized functional ($E(\Psi_a)$ or $D(\Psi_a)$) reaches the minimum.

Using this iterative procedure we shall obtain the sequence of states in which each state improves the previous one in the optimal way.

The value of the variance, which we will reach by executing the iterative cycles, is the measure of non-accuracy of the stationary state we have found. This allows us to regulate the accuracy of the calculations and provides a very useful criterion for stopping the iterative procedure. This is true also in the case of energy minimization, of course, because D is minimized simultaneously.

The Hilbert space, which will be used for solving our theory in this way, was specified in Sect. II. It is generated by the set of orthonormal states (24). Each vector of this space is characterized by the coefficients (c_K) in decomposition

$$\Psi \equiv (\dots c_{-K}, \dots c_{-1}, c_0, c_1, \dots c_K, \dots) \equiv \sum_{K=-\infty}^{\infty} \frac{c_K}{4\pi^2} \exp(\mathrm{i}K\Phi) \qquad (27)$$

where $\Phi = \varphi_1 + \varphi_2 - \varphi_3 - \varphi_4$ is the angular variable; $K = 0, \pm 1, \pm 2, \dots$

In practice we have to restrict ourselves to the finite dimensional subspace of the Hilbert space, i.e., to work with the finite number of the nonzero components of a given vector. One can notice, however, that if the initial vector $|\Psi_i\rangle$ has $2K+1$ nonzero components $(c_{-K}, \dots, c_K)$, then the vector $\hat{H}|\Psi_i\rangle$ will have $2K+3$ components $(c_{-K-1}, \dots, c_{K+1})$. It means that the gradient of $E(\Psi_i)$ and $D(\Psi_i)$ will have $2K+3$ and $2K+5$ components respectively. In this way the dimensionality of the subspace would increase in each iterative cycle, which is non-appropriate. That is why we started the determination of the eigenstates on the subspace with a lower dimensionality (about 20) and cut off the additional nonzero components. After a given accuracy of the stationary state was reached, we have increased the dimensionality of the subspace and made the calculations more accurate. We have changed the dimensionality up to 40.

For the minimization of $E(\Psi_a)$ and $D(\Psi_a)$ we have used the well-known "success-failure" one dimensional minimization method [4].

The results for the ground state are shown in Tab. 1. For a given value of g we show the energy of the ground state, which was obtained by energy minimization (E_E) and the same for the variance minimization (E_D). D_D is the variance we have reached in the latter case.

The eigenvalue problem solved here is equivalent to the determination of the eigenvalues of the Mathieu equation, which correspond to the solutions with the period of π [5]. The results are known in the form of power series in the coupling constant $q = 1/g^4$ [6]. We have used this series up to the 8th power to compare the eigenvalues with our results (see the value of E in Tab. 1), but this is usable only for the weak coupling region ($g \gtrsim 1$)[1]). One can see that in this region there is an extremely good agreement.

[1]) That is why some of the places in our tables are free.

Table 1

Ground state energies. For a given value of g there is shown the energy obtained by energy minimization (E_E) and the same for variance minimization (E_D). D_D is the variance which was reached in the latter case. E is the energy obtained from the power series for the eigenvalues of the Mathieu equation.

g	0.1	0.5	1.0	3.0
E_E	0.99945	0.96766	0.77243	0.11076
E_D		0.96768	0.77547	0.11077
E			0.77286	0.11076
D_D		0.6×10^{-4}	0.7×10^{-2}	0.1×10^{-3}

It is more remarkable, however, that the SDM provides the natural possibility of an accuracy estimate, which is not dependent on the value of the coupling constant. The rough estimate of this type is derived in the Appendix. It has the form

$$|E_k - \tilde{E}_k| \approx \tilde{D}_k \frac{|\tilde{E}_{k-1} + \tilde{E}_{k+1}|}{(\delta\tilde{E}_{k-1,k})^2 + (\delta\tilde{E}_{k,k+1})^2}, \qquad (28)$$

where $\tilde{E}_k$ is the energy of the kth approximative stationary state we have found

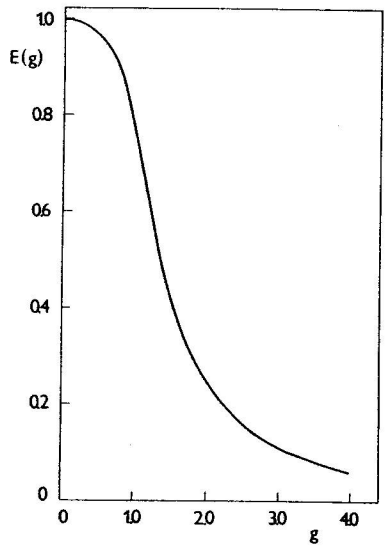

Fig. 2. The g-dependence of the ground state energy of the system.

Table 2

Excited state energies. For a given value of g are shown the energies of the first six excited states (NS — number of state). E_D is the energy of the stationary state and D_D is the value of variance we have reached. E is the energy obtained from the corresponding series for the eigenvalue of the Mathieu equation.

NS	g	0.6	0.8	1.0	3.0
2	E_D	2.75527	2.68744	2.95851	18.11105
	E		2.68743	2.95851	18.11105
	D_D	0.1×10^{-4}	0.2×10^{-4}	0.1×10^{-4}	0.6×10^{-5}
3	E_D	4.24044	3.34200	3.18533	18.11139
	E			3.18521	18.11139
	D_D	0.4×10^{-3}	0.4×10^{-3}	0.7×10^{-3}	0.4×10^{-4}
4	E_D	5.86324	6.74213	9.01648	72.11113
	E		6.74215	9.01640	72.11113
	D_D	0.3×10^{-4}	0.6×10^{-5}	0.6×10^{-5}	0.5×10^{-5}
5	E_D	6.19843	6.75160	9.01691	72.11113
	E		6.75163	9.01691	72.11113
	D_D	0.9×10^{-3}	0.2×10^{-4}	0.3×10^{-4}	0.1×10^{-4}
6	E_D	9.41146	13.10979	19.00714	162.11112
	E		13.10979	19.00714	162.11112
	D_D	0.1×10^{-5}	0.5×10^{-5}	0.2×10^{-5}	0.2×10^{-6}
7	E_D	9.41611	13.10979	19.00714	162.11112
	E		13.10980	19.00714	162.11112
	D_D	0.3×10^{-4}	0.3×10^{-4}	0.2×10^{-5}	0.9×10^{-6}

and $\tilde{D}_k$ is its variance; $\delta\tilde{E}_{i,j} = |\tilde{E}_i - \tilde{E}_j|$; E_k is the energy of the kth true stationary state. The derivation of Eq. (28) is shown in the Appendix. For $g = 0.5$ (which corresponds to $q = 16$), we have, for instance, $|E_0 - \tilde{E}_0| \approx 10^{-5}$ and for $g = 2$ ($q = 1/16$) $|E_0 - \tilde{E}_0| \approx 10^{-4}$. The latter case corresponds to the order in which the values of E_D and E differ.

The dependence of the ground state energy on the coupling constant is shown in Fig. 2.

The results for the excited states are given in Tab. 2. We have calculated the first six excited state energies of the system on the same level of accuracy as the

ground state energies. In the weak coupling region the results are compared with the eigenvalues of the Mathieu equation again. The corresponding values differ in the order indicated by Eq. (28).

Several problems arise in using the SDM to calculate the excited state. The first of them is how to identify the state we have found by variance minimization. By executing the iterative cycles we get some state with the value of variance which is near to zero, but from this point of view all the stationary states are equivalent. The second problem is connected with the previous one. According to our opinion the variance minima are very "narrow" if we compare them with the variance minimum of the ground state. That is why the variance minimization practically always leads to the ground state. One has to have some preliminary rough information about the structure of the excited states to reach its variance minima.

In this special case these problems can be easily solved by using the following strategy:

From Eq. (23) it can be seen immediately that in the $g \to \infty$ limit our basis functions correspond to the eigenfunctions of the hamiltonian. This means that if we start our calculations with the large value of g, we will know the structure of a given excited state and will be able to identify it. The stationary state will be obtained very quickly and we will use it as an initial variational state for the hamiltonian with g somewhat smaller than in the previous case. If we suppose the continuous dependence of $E(g)$ for a given stationary state, then it is natural

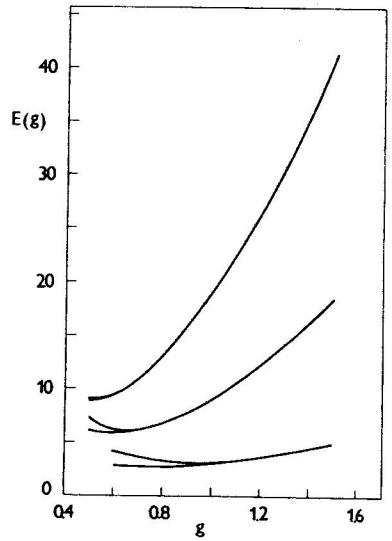

Fig. 3. The g-dependence of the first six excited states of the system.

to expect that this variational state will be very "near" to the true stationary state and the identification will be conserved. By the repetitive usage of such a quasi-continuum shift in g we can investigate the spectrum in the large range of values of g, including the strong coupling region.

To identify the spectrum in this way exactly one has to use the property of symmetry of the hamiltonian. It can be seen immediately that the hamiltonian (23) is invariant with respect to the transformation $\Phi \to -\Phi$. This means that the eigenfunctions, corresponding to a given value of energy, can be symmetrized and antisymmetrized. As a consequence we have in the $g \to \infty$ limit the double degeneracy of the excited states. That is why we have shifted so the symmetric state as the antisymmetric one to the strong coupling region. In this region the degeneracy is removed (see Fig. 3.).

IV. CONCLUSIONS

We have tested here the steepest descent method on a simple U(1) theory on a lattice with a single plaquette in the 2 + 1 dimensions. The ground and a few excited states were determined and identified for various values of the coupling constant. The results are very accurate and very easy to obtain even for the excited states.

The realization of the method we have used is very effective and gives the change to calculate the nonperturbative effects of the theory. We hope that method could be used also in more realistic cases, including the quantum theory of fields.

ACKNOWLEDGEMENT

The author is indebted to V. Černý, I. Novák and J. Pišút for their useful recomendations and to J. Ftáčnik, Š. Olejník and J. Pišút for reading the manuscript.

APPENDIX

We shall derive here the estimate (28).

Let us suppose that we have found the approximative state $|\tilde{\Psi}_k\rangle$ to the kth true stationary state. It means that the value of variance $\tilde{D}_k$ is small in this state. We are interested in the order of accuracy for the corresponding eigenenergy $\tilde{E}_k$.

The variance of the hamiltonian can be written in the form

$$\tilde{D}_k = \sum_{i=1}^{\infty} |c_i|^2 E_i^2 - \left(\sum_{i=1}^{\infty} |c_i|^2 E_i \right)^2, \tag{29}$$

where E_i are the eigenenergies of the hamiltonian and c_i are the components of $|\tilde{\Psi}_k\rangle$ in the eigenfunction representation. As $|\tilde{\Psi}_k\rangle$ approximates the kth stationary state, the relations

$$|c_i| \ll |c_k|, \qquad i \neq k \tag{30}$$

are satisfied.

To get the rough estimate of the accuracy of $\tilde{E}_k$ we shall suppose that c_{k-1}, c_k, c_{k+1} are the only nonzero components of $|\tilde{\Psi}_k\rangle$. Due to Eq. (30) the terms $|c_i|^2 c_j|^2$ for $i, j = k-1, k+1$ can be neglected in (29), which leads to

$$\tilde{D}_k \approx |c_k|^2 [|c_{k-1}|^2 (\delta E_{k,k-1})^2 + |c_{k+1}|^2 (\delta E_{k+1,k})^2, \tag{31}$$

where $\delta E_{i,j} = |E_i - E_j|$.

If we put in (31) approximatively $|c_k|^2 \approx 1$, $|c_{k-1}| \approx |c_{k-1}| = c$, then we will obtain

$$c \approx \frac{\tilde{D}_k}{(\delta E_{k-1,k})^2 + (\delta E_{k+1,k})^2}. \tag{32}$$

Using this expression we shall find immediately

$$|\tilde{E}_k - E_k| \approx \left| \sum_{i=k-1}^{k+1} |c_i|^2 E_i - E_k \right| \approx \tilde{D}_k \frac{|E_{k-1} + E_{k+1}|}{(\delta E_{k-1,k})^2 + (\delta E_{k,k+1})^2} \tag{33}$$

The substitution of the approximative eigenenergies $\tilde{E}_k$ into the right-hand side of Eq. (33) reproduces the result (28).

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Received September 23rd, 1988
Accepted for publication November 23rd, 1988