

New look at the Lanczos method in the lattice gauge model

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Abstract. In the present work we combine the Lanczos algorithm and the lowest order constrained variational method (LOCV) to obtain a simple version of the Lanczos algorithm. In order to test the method the ground state energy and the antisymmetric mass gap of the U(1) lattice gauge model are calculated, and the results are compared with those computed by other many body methods.

1 Introduction and review

The Lanczos technique is a powerful method for tridiagonalizing the large matrices, specially sparse ones, in order to find their spectra. It may provide a sequence of approximations which rapidly converges to the eigenvalues of the matrices [1, 2].

It is a very suitable method when one needs to calculate the lowest eigenvalues of the Hamiltonian of a many body system, because it uses only relatively few states from the full Hilbert space of the system [3–5].

The Lanczos method, like the other variational methods, gives us an upper bound to the true ground state energy:

$$E_g \leq E[\psi_{\text{trial}}] = \frac{\langle \psi_{\text{trial}} | H | \psi_{\text{trial}} \rangle}{\langle \psi_{\text{trial}} | \psi_{\text{trial}} \rangle}. \quad (1)$$

The main idea of the Lanczos method is based on the fact that the trail state, i.e. $|\psi_{\text{trail}}\rangle$, can be written as

$$|\psi_{\text{trail}}\rangle = \sum_{n=0}^m \alpha_n |\psi_n\rangle = \sum_{n=1}^m a_n H^{n-1} |\psi_1\rangle, \quad (2)$$

where $|\psi_1\rangle$ is a seed state for generating m -dimensional orthonormal basis states, i.e. $\{|\psi_n\rangle\}$, in an iterative procedure as follows:

$$|\psi_n\rangle = H|\psi_{n-1}\rangle - \gamma|\psi_{n-1}\rangle - \beta|\psi_{n-2}\rangle. \quad (3)$$

The coefficients γ and β are determined in each iteration step by imposing the normalization and orthogonality conditions on the basis states,

$$\langle \psi_n | \psi_n \rangle = 1, \quad (4)$$

$$\langle \psi_n | \psi_{n-1} \rangle = \langle \psi_n | \psi_{n-2} \rangle = 0. \quad (5)$$

If m goes to infinity the above basis can span the whole Hilbert space. Then the Hamiltonian is completely tridiagonalized and the exact eigenvalues are computed via

the standard procedure. But for a finite value of m , i.e. the case that we face in practical problems, only an m -dimensional subset of the Hamiltonian will be tridiagonalized.

However, if we expect to approximate the lowest levels of the energy spectrum, it would be sufficient to evaluate them by finding the eigenvalues of the tridiagonalized finite-dimensional subset of the Hamiltonian.

The Lanczos method may be presented in the form of various kinds of algorithms [3, 6, 7] but the above presentation is well known.

Although the advantages of the Lanczos method are clear, it faces a few serious problems.

- (i) The appearance of spurious eigenvalues in practice when the number of iterations becomes large.
- (ii) In many body problems or field theories, after the application of the Hamiltonian in each subsequent step in an iteration a large number of independent structures appear which should be treated as different states. Therefore, the number of the states in the basis grows rapidly as the iteration procedure proceeds.

There are two ways to solve the first problem [8, 9]. Both are based on an algorithm for finding and omitting spurious eigenvalues, but we should expect making costs in terms of computation time.

The second problem can be solved by a reduction of the states which are arising in the iteration procedure. One way is reduction of the Hilbert space similar to the idea that lies behind the density matrix renormalization group technique [10]. Here we present a simple and systematic reduction of the basis states by combining the lowest order constrained variational (LOCV) method [11–13] and the Lanczos algorithm.

The LOCV method has been developed and extended during the past two decades by one of us (MM) to study the properties of various quantum fluids, such as nuclear and neutron matter. This technique is based on the mini-

mization of the energy, which usually comes from the lowest order cluster expansion, with respect to a suitable trial state and a constraint in order to take into account the effects of the higher order terms in the cluster expansion of the energy.

We present in Sect. 2 the formalism of LOCV and the way we will merge it to the Lanczos algorithm. Section 3 is devoted to the application of a combined method to the well-known problem, the U(1) gauge model. Thus the ground state energy and the antisymmetric mass gap are computed. We summarize our work in Sect. 4, focussing on a comparison of our results and those which have been obtained by other many body methods.

2 Formalism

In the cluster expansion method the trial state is obtained by application of the correlation operator F on a seed state, i.e. $|\psi_1\rangle$:

$$|\psi_{\text{trail}}\rangle = F(1, 2, \dots, N)|\psi_1\rangle. \quad (6)$$

The seed state describes the system in the absence of any interaction, namely it may be the product of the one particle states. The operator F is symmetric and shows all of the correlations between the system constituents. The correlation operator has the cluster property; it will become a product of two factors if the system decomposes in two pieces (clusters) with n and $N - n$ particles, respectively, such that there would not be any interaction between them,

$$F(1, 2, \dots, N) \rightarrow F_n(1, \dots, n)F_{N-n}(n+1, \dots, N). \quad (7)$$

The first three terms in the cluster expansion of energy is usually written in the following form [14]:

$$E_1 = \langle \psi_1 | T(1) | \psi_1 \rangle, \quad (8)$$

$$E_2 = \frac{1}{2} \langle \psi_1 | \frac{1}{2} F_2^\dagger(1, 2) [T(1) + T(2), F_2(1, 2)] + \text{adj.} \\ + F_2^\dagger(1, 2) V(1, 2) F_2(1, 2) | \psi_1 \rangle \quad (9)$$

and

$$E_3 = \frac{1}{3!} \langle \psi_1 | \frac{1}{2} F_3^\dagger(1, 2, 3) [T(1) + T(2) + T(3), \\ F_3(1, 2, 3)] + \text{adj.} + F_3^\dagger(1, 2, 3) \{V(1, 2) + V(2, 3) \\ + V(1, 3)\} F_3(1, 2, 3) | \psi_1 \rangle \\ - E_2 \langle \psi_1 | F_2^\dagger(1, 2) F_2(1, 2) | \psi_1 \rangle, \quad (10)$$

where $T(1)$ and $V(1, 2)$ are the one and two particle parts of the Hamiltonian, respectively, i.e.

$$H = \sum_n T(n) + \sum_{m < n} V(m, n). \quad (11)$$

In the LOCV method we impose a constraint on the correlation operators and minimize (9) with respect to them by introducing a Lagrange multiplier,

$$\frac{\delta E_2[F_2(1, 2)]}{\delta F_2(1, 2)} - \mu \frac{\delta C[F_2(1, 2)]}{\delta F_2(1, 2)} = 0. \quad (12)$$

The choice of the constraint $C[F_2(1, 2)]$ is very important. Beside that it should have physical meaning, it would have to make the convergence of the cluster series as fast as possible. It is well known that the normalization constraint [15] satisfies both above conditions, i.e.,

$$C[F_2(1, 2)] = \langle \psi_1 | F_2^\dagger(1, 2) F_2(1, 2) - 1 | \psi_1 \rangle = 0. \quad (13)$$

Equation (10) is used to check the plausibility of the LOCV results.

We use the idea of the Lanczos method to define the correlation operator F as follows:

$$F = \sum_{n=1}^m a_n H^{n-1}. \quad (14)$$

The above adoption of the correlation operator can be applied to the LOCV method in (12),

$$E = \frac{\sum_{q=1}^m \sum_{p=1}^m a_q a_p \langle \psi_1 | H^{q+p}(1, 2) | \psi_1 \rangle}{\sum_{q=1}^m \sum_{p=1}^m a_q a_p \langle \psi_1 | H^{q+p-1}(1, 2) | \psi_1 \rangle}. \quad (15)$$

The coefficients $\{a_n\}$ are determined by the same procedure, namely the Lanczos algorithm which was described previously.

In the following section we apply the above reduced version of the Lanczos method to the well-known problem of the U(1) lattice gauge model.

3 The U(1) model

We can extract all physical properties of the U(1) lattice gauge model in two dimensions from the Hamiltonian which is usually written as

$$H = \sum_X \left\{ -2 \frac{\partial^2}{\partial B_X^2} + \lambda(1 - \cos B_X) \right\} \\ + \frac{1}{2} \sum_{X, \rho} \frac{\partial^2}{\partial B_X \partial B_{X+\rho}}, \quad (16)$$

where X labels the plaquettes of the lattice, ρ represents the unit vectors in the principal directions and B_X is an angle variable ($-\pi \leq B_X \leq \pi$) which is called the magnetic field of the plaquette X .

The different phases of the system are characterized by a positive and dimensionless coupling constant λ . We acquire the strong (weak) coupling phase when the coupling constant approaches zero (infinity).

The Hamiltonian is invariant under the reflection transformation $X \rightarrow -X$; therefore, it should have symmetric and antisymmetric branches of the eigenvalues.

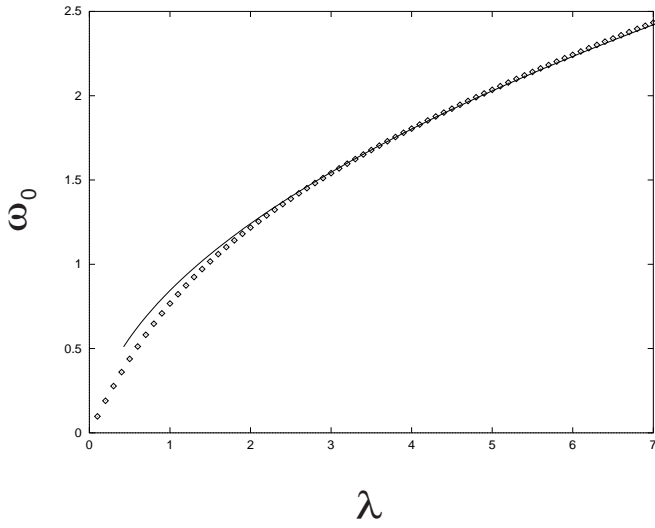


Fig. 1. The ground state energy per plaquette of the U(1) lattice gauge as a function of the coupling constant. The solid line represents the perturbation expansion form for the weak coupling limit, and the points display our result

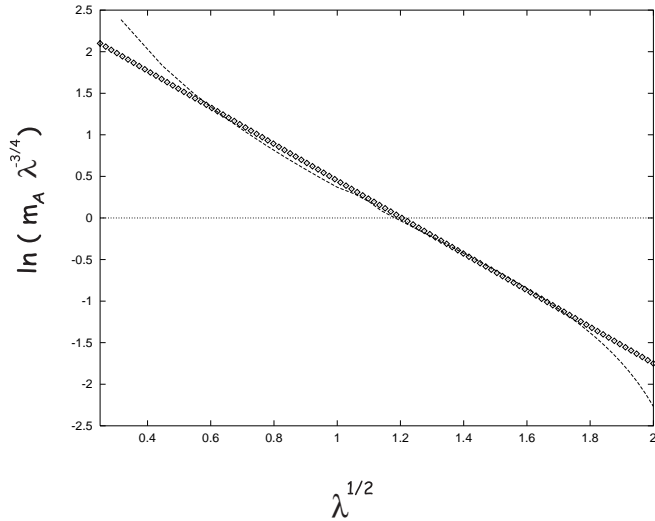


Fig. 2. The logarithm of antisymmetric mass gap as a function of the squared root of coupling constant. The solid line is the result of fitting for $1.2 < \lambda^{1/2} < 1.78$ to find the unknown parameters in the weak coupling limiting form (19)

Here we are interested in the calculation of the ground state energy density ω_0 and the density of the first antisymmetric energy excitation ω_A . The corresponding measurable quantity, the antisymmetric mass gap is the difference between these values,

$$m_A = \omega_A - \omega_0. \quad (17)$$

To compute the above quantities, in the first step we should evaluate the moments of the Hamiltonian $\{\langle H^n(1,2) \rangle\}$. We choose $|0\rangle$ and $(\sin B_1 + \sin B_2)|0\rangle$ as our symmetric and antisymmetric seed state. The state $|0\rangle$ expresses that the magnetic field of all plaquettes is equal to zero.

Table 1. Results for the coefficients α_0 and α_1 in the weak coupling limit for the photon mass gap

Sources	α_0	α_1
Villain [21]	2.49	2.18
BRG [24]	2.05	2.49
MC [23]	2.65	3.07
CBF [18]	2.40	3.13
CCM [17]	2.50	2.94
BTE [19]	2.61	2.97
LOCV [22]	2.40	2.89
Present work	2.20 ± 0.03	2.65 ± 0.05

The result of our calculation for the ground state energy density is shown in Fig. 1. This is in fair agreement with the results that were obtained by other many body techniques [16–19, 22]. The perturbation expansion form for the weak coupling limit [20] can also be given:

$$\omega_0 = 0.958\sqrt{\lambda} - 0.114 + \dots (\lambda \rightarrow \infty). \quad (18)$$

The behavior of the logarithm of the photon mass as a function of the squared root of the coupling constant is displayed in Fig. 2. The photon mass gap has the following asymptotic form in the weak coupling limit [21]:

$$m_A = \lambda^{3/4} e^{-\alpha_0\sqrt{\lambda} + \alpha_1}. \quad (19)$$

Many authors reported numerical values for α_0 and α_1 in the above equation. Our results for these coefficients which are obtained by fitting to the weak coupling asymptotic form in (19) for $1.2 < \lambda^{1/2} < 1.78$ are given in Table 1. The other [17–19, 22–24] calculations are also presented for comparison.

We can check the consistency of our combined method by considering the remaining terms in the energy cluster expansion. To find the third order correction to the energy we should mention here that in the above calculation we have restricted ourselves to the two plaquette approximation. Then the three plaquette correlation operator is written as a sum of two plaquette correlation operators,

$$F_3(1, 2, 3) = F_2(1, 2) + F_2(2, 3) + F_2(1, 3), \quad (20)$$

and it is clear from (10) that the third order energy correction is equal to zero.

The plausibility of a two plaquette approximation is checked by comparison of our results with those which are carried out by other many body methods as we did before.

4 Summary

The Lanczos method is a powerful tool for solving many body problems but in practical applications of this method we encounter a large number of basis states which are obtained in each step of iteration.

For example in the case of the U(1) lattice gauge model we have in the fourth, fifth and sixth steps of the iteration 67, 357 and 2457 basis states, respectively [17]. As regards the consumption of the calculation time and the number of bytes in memory we should choose the more important states among the set of all basis states.

The lowest order constrained variational method offers a simple and a systematic way to sieve the basis states. To have a comparison we must note that in the case of a U(1) model the number of states is reduced to 71 in the sixth iterations step.

The results which are obtained for the ground state energy and the antisymmetric mass gap are comparable with other results.

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