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Variational Wavefunctions for Non-compact U(1) Lattice Gauge Theory: Comparison with Exact Result

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Abstract

Estimates of the ground state wavefunction of (2+1)-dimensional non-compact U(1) Hamiltonian lattice gauge theory are found in terms of variational wavefunctions with up to four parameters. These wavefunctions are compared with the exact ground state as a test of the accuracy of the method.

1. Introduction

An interesting alternative to the standard Euclidean path integral techniques of lattice gauge theory is provided by the method of variational wavefunctions. In this method, one deals with the Hamiltonian formalism and realises the states of the system as functionals of lattice link variables. By minimising the expectation value of the lattice Hamiltonian with respect to a finite number of parameters in a trial wavefunction, an estimate of the true ground state is found. This method has been applied to both Abelian and non-Abelian gauge theories. Compact U(1) gauge theory in (2+1) dimensions has been studied by Heller (1981), Heys and Stump (1987) and Dabringhaus *et al.* (1991), while SU(2) gauge theory has been studied in (2+1) dimensions by Arisue *et al.* (1983) and in (3+1) dimensions by Heys and Stump (1984) and Horn and Karliner (1984). Of more relevance to QCD are the SU(N) results of Chin *et al.* (1986) and Long *et al.* (1988), which are summarised in Robson *et al.* (1988). Their calculations of glueball masses and the string tension show a reasonable consistency with Euclidean Monte Carlo results.

In this paper we apply the method to a simple exactly solvable model, namely non-compact U(1) gauge theory in (2+1) dimensions (Drell *et al.* 1979). The model is equivalent to the lattice version of a free Klein–Gordon field, for which the full spectrum of energy eigenstates can easily be found. This enables us to compare not only the estimate of the ground state energy with the exact value, but also to test the accuracy of the variational wavefunction itself. In Section 2 we give the analytic solution for the ground state of (2+1)-dimensional non-compact U(1) lattice gauge theory and describe the trial wavefunctions used in our subsequent numerical calculations. Results of the numerical calculations are given in Section 3, and our conclusions summarised in Section 4.

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2. Non-compact U(1) in (2+1) Dimensions

We begin with the dimensionless lattice Hamiltonian

$$W = -\sum_l \frac{\partial^2}{\partial\theta_l^2} + x\sum_p \theta_p^2, \tag{1}$$

where the variables θ_l defined on the links of a two-dimensional square lattice take values in the range $(-\infty, \infty)$ and the plaquette variables

$$\theta_p = \theta_{l_1} + \theta_{l_2} - \theta_{l_3} - \theta_{l_4} \tag{2}$$

are defined in terms of the links bounding the plaquette p. The naive continuum limit is obtained from

$$H = \frac{e^2}{2}W \to \tfrac{1}{2}\int (\mathbf{E}^2 + B^2) d^2\mathbf{r} \tag{3}$$

by making the substitutions

$$x = \frac{1}{e^4 a^2}, \qquad \theta_l \to eaA_i(\mathbf{r}), \qquad i\frac{\partial}{\partial\theta_l} \to ae^{-1}E^i(\mathbf{r}), \tag{4}$$

where e is the (dimensionful) electric charge and a the lattice spacing.

The compact version, obtained by replacing the magnetic term in equation (1) by $2x\,\Sigma_p\,(1-\cos\theta_p)$, has been studied extensively by Heys and Stump (1987) using variational wavefunctions. They report excellent agreement with an earlier Green function Monte Carlo calculation of the ground state energy (Heys and Stump 1983) by using up to six parameters in their trial wavefunction. However, they point out that the ground state energy, by itself, is not necessarily a good measure of how closely the variational wavefunction approximates the unknown true ground state.

By contrast, the non-compact version of the theory is quadratic, and therefore exactly solvable. This allows us to compare the variational wavefunction itself, as well as the ground state energy, with an exact result. Using (2) to eliminate the link variables in terms of plaquette variables, the Hamiltonian (1) can be written as a lattice Klein–Gordon Hamiltonian on the dual lattice:

$$W = \sum_{m,n} \Delta_{mn} \frac{\partial^2}{\partial\theta_m \partial\theta_n} + x\sum_m \theta_m^2, \tag{5}$$

where (Dabringhaus *et al.* 1991)

$$\Delta_{mn} = \begin{cases} -4 & \text{if } m = n, \\ 1 & \text{if } m \text{ and } n \text{ are nearest neighbours,} \\ 0 & \text{otherwise,} \end{cases} \tag{6}$$

and m, n label the sites of the dual lattice, corresponding to the plaquettes of the original lattice. We also note that the inverse coupling x can be set to 1 from this point by the rescaling $W_{\text{new}} = x^{-1/2} W_{\text{old}}$, $\theta_{\text{new}} = x^{\frac{1}{4}} \theta_{\text{old}}$ in (5).

Taking the lattice to be square periodic of size $N \times N$, the Hamiltonian (5) is diagonalised by the finite Fourier transform

$$\tilde{\theta}_k = \frac{1}{N} \sum_{n_1, n_2} e^{(2\pi i/N)(k_1 n_1 + k_2 n_2)} \theta_n \,, \tag{7}$$

where we have labelled the sites of the coordinate and momentum space lattices $n = (n_1, n_2)$ and $k = (k_1, k_2)$ respectively, and where $n_i, k_i = 0, \ldots, N-1$. The diagonalised Hamiltonian is then

$$W = \sum_k \left(- \Lambda_k \frac{\partial^2}{\partial \tilde{\theta}_k^* \partial \tilde{\theta}_k} + \tilde{\theta}_k^* \tilde{\theta}_k \right), \tag{8}$$

where

$$\Lambda_k = 4 \left(\sin^2 \frac{\pi k_1}{N} + \sin^2 \frac{\pi k_2}{N} \right). \tag{9}$$

This is clearly a sum of uncoupled harmonic oscillators, corresponding to the photon excitations of the lattice. The ground state energy per plaquette of the original lattice is then

$$E_0 = \frac{1}{N^2} \sum_k \Lambda_k^{\frac{1}{2}} = \frac{2}{N^2} \sum_k \left(\sin^2 \frac{\pi k_1}{N} + \sin^2 \frac{\pi k_2}{N} \right)^{\frac{1}{2}}, \tag{10}$$

and the ground state wavefunctional

$$\Psi_0[\theta] = \mathcal{N} \left[\delta \left(\sum_n \theta_n \right) \right]^{\frac{1}{2}} \exp \left(- \tfrac{1}{2} \sum_{m,n} \theta_m M_{mn} \theta_n \right), \tag{11}$$

where

$$M_{mn} = \frac{1}{N^2} \sum_{k \neq (0,0)} e^{-(2\pi i/N)[k_1(m_1 - n_1) + k_2(m_2 - n_2)]} \Lambda_k^{-\frac{1}{2}} \,, \tag{12}$$

and $\mathcal{N}$ is an uninteresting normalisation factor. The delta function in (11) arises from the $k = 0$ mode in the diagonalised Hamiltonian (8). This solution has been used by Drell *et al.* (1979) as a starting point for estimating the ground state of the compact version of the theory.

Because of translation and reflection symmetry of the ground state, it is clear that not all of the matrix elements M_{mn} specifying the state are independent. Setting

$$\beta_n^{\text{exact}} = M_{0n} \tag{13}$$

(so that $M_{mn} = \beta^{\text{exact}}_{n-m}$), we see that the ground state is completely specified by the $\frac{1}{2}([N/2]+1)([N/2]+2)$ numbers $\beta^{\text{exact}}_{(n_1,n_2)}$, where $[N/2] \geq n_1 \geq n_2 \geq 0$.

We wish to estimate this ground state by a variational wavefunction with only a small number of free parameters. Keeping within the spirit of the wavefunctions based on Wilson loops used by Heys and Stump (1987), an obvious gauge invariant choice of trial wavefunction is

$$\Psi_{\mathrm{T}}[\theta] = \exp\left(-\tfrac{1}{2} \sum_{L} \alpha_L \Phi_L^2 \right), \tag{14}$$

where the sum is over a restricted set of loops L in the original lattice and Φ_L is the oriented sum of link variables around each loop L:

$$\Phi_L = \sum_{l \in L} (\pm) \theta_l \,. \tag{15}$$

In (15) the plus (minus) sign is taken if the link is traversed in the positive (negative) direction when going round the loop in an anticlockwise direction. The set of loops will typically contain all loops up to a given size, for example, all loops bounding up to three connected plaquettes.

Obviously the trial wavefunction (14) can only give rise to quadratic terms in plaquette variables in the exponent. An equivalent specification of trial wavefunctions is therefore given in terms of sites on the dual lattice by

$$\Psi_{\mathrm{T}}[\theta] = \exp\left(-\tfrac{1}{2} \sum_{mn} \theta_m \beta_{n-m} \theta_n \right), \tag{16}$$

where the β are only nonzero for a small set of site separations $m-n$. For example, a three-parameter Ψ_{T} may be restricted to include only self interactions $\beta_{(0,0)}$, nearest neighbour interactions $\beta_{(1,0)}$ and nearest diagonal neighbour interactions $\beta_{(1,1)}$. The β values are fixed by minimising the expectation value of the Hamiltonian (5):

$$\frac{\langle \Psi_{\mathrm{T}} \,|\, W \,|\, \Psi_{\mathrm{T}} \rangle}{\langle \Psi_{\mathrm{T}} | \Psi_{\mathrm{T}} \rangle} =$$

$$\int \prod_n d\theta_n \left[-\sum_{m,n} \beta_{n-m} \Delta_{mn} + \sum_{m,n,r,s} \theta_r \beta_{m-r} \Delta_{mn} \beta_{s-n} \theta_s + \sum_n \theta_n^2 \right]$$

$$\times \frac{e^{-\sum \theta_m \beta_{n-m} \theta_n}}{\int \prod_n d\theta_n e^{-\sum \theta_m \beta_{n-m} \theta_n}} \,. \tag{17}$$

Provided the nonzero β only include a small number of short-range interactions, the integral is readily done in the computer by a Monte Carlo simulation. In the following numerical calculations, Monte Carlo ensembles were generated for wavefunctions containing the full set of nonzero β values in the trial wavefunction.

This contrasts with the non-compact U(1) calculations of Heys and Stump (1987), who simplified their numerical calculations by drawing their Monte Carlo ensembles from a one-parameter subset of parameter space.

3. Numerical Results

Our numerical simulations were done on 8×8 and 16×16 lattices with variational wavefunctions containing up to 4 parameters in the 8×8 case and 3 parameters in the 16×16 case. Calculations were also done using a 3×3 lattice, for which the exact ground state contains only three parameters, in order to test the computer code. Using a Metropolis algorithm, the θ_n were chosen from the range -8 to 8. Given that fewer than 1 in 100 accepted values were outside the range $-2{\cdot}5$ to $2{\cdot}5$, we considered this to be a very safe domain which would still see a reasonable turnover of values. Beginning from a random initial configuration, each site was updated 5 times per sweep and the first 500 sweeps discarded. The sample was then taken from every third sweep for the larger lattices, and every sixth sweep for the 3×3 lattice. To locate the miminum of the ground state energy $\langle W \rangle$ in parameter space, first a broad scan of the expected region was made to locate the approximate minimum, and then a more careful scan using far higher statistics was performed in the immediate vicinity. The final values quoted below are obtained by minimising a quadratic fit to $\langle W \rangle$ as a function of the β values.

Comparing the exact ground state wavefunction (11) with the trial wavefunction (16), it is clear that the variational parameters β would be directly analogous to the parameters β^{exact} defined by (13), were it not for the δ-function occurring in (11). The effect of the δ-function can be thought of as adding an infinite constant to each of the $\beta^{\text{exact}}_{n-m}$. To illustrate this, consider the 3×3 lattice, for which the exact ground state is given by (11) and (13) with

$$\beta^{\text{exact}}_{(0,0)} = \frac{4+2\sqrt{2}}{9\sqrt{3}} \approx 0{\cdot}438044\,,$$

$$\beta^{\text{exact}}_{(1,0)} = \frac{1-\sqrt{2}}{9\sqrt{3}} \approx -0{\cdot}026572\,,$$

$$\beta^{\text{exact}}_{(1,1)} = \frac{\sqrt{2}-4}{18\sqrt{3}} \approx -0{\cdot}082939\,, \tag{18}$$

and ground state energy per plaquette

$$E_0^{3\times 3} = \frac{4(1+\sqrt{2})}{3\sqrt{3}} \approx 1{\cdot}858462\,. \tag{19}$$

Searching the parameter space for the minimum energy of the three-parameter trial wavefunction Ψ_T using the Monte Carlo procedure outlined above, we were not able to locate a minimum at finite β. Instead we found a long, downward sloping valley approximately following the line

$$(\beta_{(0,0)}, \beta_{(1,0)}, \beta_{(1,1)}) = (\beta^{\text{exact}}_{(0,0)} + \lambda, \beta^{\text{exact}}_{(1,0)} + \lambda, \beta^{\text{exact}}_{(1,1)} + \lambda)\,. \tag{20}$$

Table 1. Estimates of the ground state energy $\langle W \rangle$ of the 3 × 3 lattice calculated from equation (17) using the β parameters given by (20)

The numbers in parentheses in this and the subsequent tables are the numerical uncertainty in the last digits

λ	$\langle W \rangle$	λ	$\langle W \rangle$
1·0	1·861548(9)	5·0	1·8590797(18)
2·0	1·860009(5)	6·0	1·85889772(15)
3·0	1·8594957(35)	7·0	1·8589037(12)
4·0	1·8592322(26)	10·0	1·85877

Table 2. Estimates of the ground state energy $\langle W \rangle$ of the 3 × 3 lattice calculated from equation (17) with $\beta = \beta^{\text{exact}}$ and a cutoff $|\sum_n \theta_n| \leq K$

The percentage of generated sweeps satisfying the cutoff criterion is also given

K	Acceptance rate	$\langle W \rangle$
0·08	1·23%	1·86060(3)
0·04	0·61%	1·858997(7)
0·02	0·31%	1·8585976(17)
0·01	0·16%	1·8584960(4)

Table 3. Minimum energy $\langle W \rangle$ and β-parameters for the variational wavefunctions (16) on an 8 × 8 lattice

The 1-parameter results are from an analytic calculation and the 2-, 3- and 4-parameter results from Monte Carlo simulations. Also given are the results of imposing a cutoff $|\sum_n \theta_n| \leq K$ to model the δ-function in (10) and the exact results for 8 × 8 and infinite lattices from (11) and (13)

	$\langle W \rangle$	(% above E_0)	$\beta_{(0,0)}$	$\beta_{(1,0)}$	$\beta_{(1,1)}$	$\beta_{(2,0)}$	$\beta_{(2,1)}$
1 param	2	(+4·5%)	0·50				
2 param	1·93739(10)	(+1·26%)	0·5476(30)	0·0628(10)			
3 param	1·9270(8)	(+0·71%)	0·5728(50)	0·0862(20)	0·0314(10)		
4 param	1·92367(30)	(+0·54%)	0·5752(40)	0·0934(20)	0·0338(20)	0·0148(20)	
3 param ($K = 0·01$)	1·91929(20)	(+0·31%)	0·5630(30)	0·0816(30)	0·0274(20)		
4 param ($K = 0·01$)	1·91696(30)	(+0·19%)	0·5784(60)	0·0940(40)	0·0332(50)	0·0146(60)	
Exact 8 × 8	1·913348		0·565348	0·087012	0·028898	0·007984	−0·004238
Exact infinite	1·916183		0·642882	0·163836	0·105070	0·082510	0·069810

Table 4. Minimum energy $\langle W \rangle$ and β-parameters for the variational wavefunctions (16) on a 16 × 16 lattice

The 1-parameter results are from an exact analytic calculation and the 2- and 3-parameter results from Monte Carlo simulations. Also given are the exact results for 16 × 16 and infinite lattices from Eqs.(11) and (13)

	$\langle W \rangle$	(% above E_0)	$\beta_{(0,0)}$	$\beta_{(1,0)}$	$\beta_{(1,1)}$	$\beta_{(2,0)}$	$\beta_{(2,1)}$
1 param	2	(+4·4%)	0·50				
2 param	1·93753(30)	(+1·13%)	0·548(2)	0·0626(10)			
3 param	1·92688(20)	(+0·58%)	0·5686(30)	0·0862(20)	0·0306(12)		
Exact 16 × 16	1·915831		0·604092	0·125134	0·066454	0·044078	0·031458
Exact infinite	1·916183		0·642882	0·163836	0·105070	0·082510	0·069810

The values of the energy obtained from (17) as λ increases, given in Table 1, appear to be converging on the correct value given in (19). Alternatively, one might try implementing the effect of the δ-function by the more obvious technique of including in the statistical ensemble only Monte Carlo updates for which $|\sum_n \theta_n|$ is less than some cutoff K. In Table 2 we show the results of calculating the ground state energy at β^{exact} as K is gradually decreased. Once again, the values obtained converge to the exact value (19).

We now turn our attention to the results for the larger lattices. In Table 3 we give the results for the 8×8 lattice, using up to 4 parameters, and in Table 4 the 16×16 lattice results using up to 3 parameters. Also listed are the values of β^{exact} for finite and infinite lattices. The variational and exact ground state wavefunctions are illustrated in Figs 1 and 2 by plotting the β-parameters against the radial distance $(n_1^2 + n_2^2)^{\frac{1}{2}}$ between plaquettes.

Immediately noticeable is that the variational parameters obtained by minimising the expectation value (17) do not differ significantly between the 8×8 and 16×16 lattices, even though the exact values β^{exact} have clearly moved closer to the infinite lattice values. This is not surprising given that the trial wavefunctions considered are localised to within a range of two lattice spacings, so the lattices used for these simulations are seen by the wavefunctions as essentially infinite. This observation is consistent with the comment made in the conclusions of Robson *et al.* (1988), namely that finite-size effects caused by the smallness of their lattices was not a serious problem, probably because of the crudeness of the wavefunctions considered. The glueball mass calculations of Long *et al.* (1988), for example, used two-parameter wavefunctions involving six link loops and were done on a 4^3 lattice. Were it possible to continue increasing the number of parameters in our 16×16 lattice simulations, we expect the β values obtained would continue to drift upwards and agree well with β^{exact} at around 9 or 10 parameters, at which point (see Fig. 2) the next parameter, $\beta^{\text{exact}}_{(3,3)}$, is close to zero.

Also given in Table 3 are the results obtained when a cutoff $|\sum_n \theta_n| \leq 0{\cdot}01$ is imposed on the Monte Carlo ensemble to model the δ-function in the exact ground state (11). Because of the extra computer time needed this was only done for the 8×8 lattice. As pointed out for the 3×3 case, the δ-function can also be accounted for by adding a large constant to each β_n, though this would clearly defeat the purpose of the Monte Carlo method which requires that only short-range interactions be nonzero. We see that the estimate of the ground state energy is improved for both the 3- and 4-parameter trial wavefunctions. However, little change is noticed in the β-parameters; the 3-parameter values show a general trend toward the exact values, whereas the 4-parameter values are unchanged. The situation seems to be similar to the 3×3 case in that there appears to be a downward sloping valley approximately following the line $\beta_n^{\text{exact}} + \lambda$ through parameter space, so that β^{exact} can be well approximated by minimising $\langle W \rangle$ over a cross section running across the valley at $\lambda = 0$. We conclude from this that once enough parameters are included in the trial wavefunction to allow for the finite lattice size, there is little advantage to be gained by imposing the cutoff at the time-consuming stage of scanning parameter space to locate the ground state.

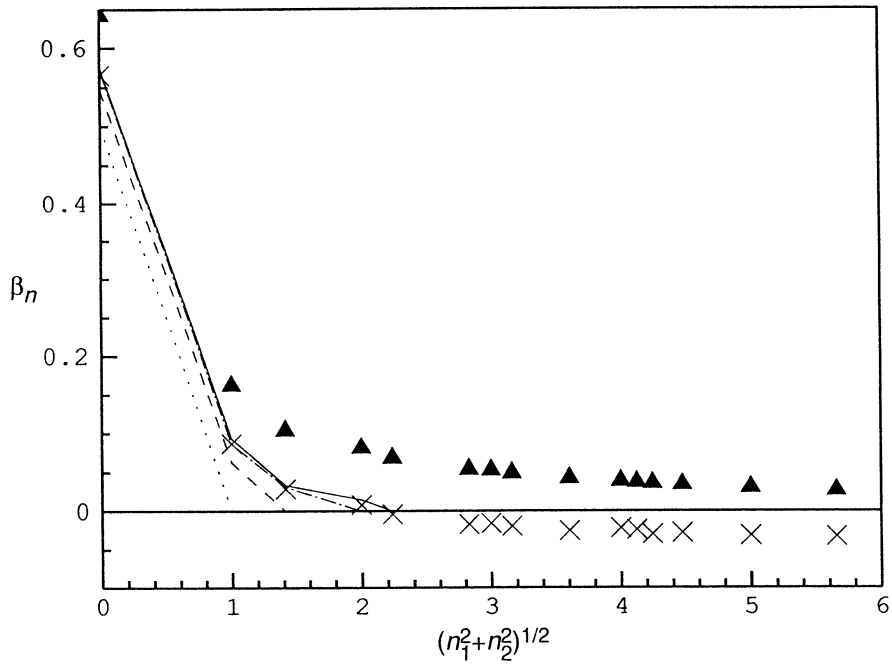

Fig. 1. Variational wavefunctions obtained by minimising equation (17) on an 8 × 8 lattice using 1 parameter (dotted line), 2 parameters (dashed line), 3 parameters (dash–dot line) and 4 parameters (solid line). The exact ground state wavefunctions on an 8 × 8 (crosses) and infinite (triangles) lattice are also shown.

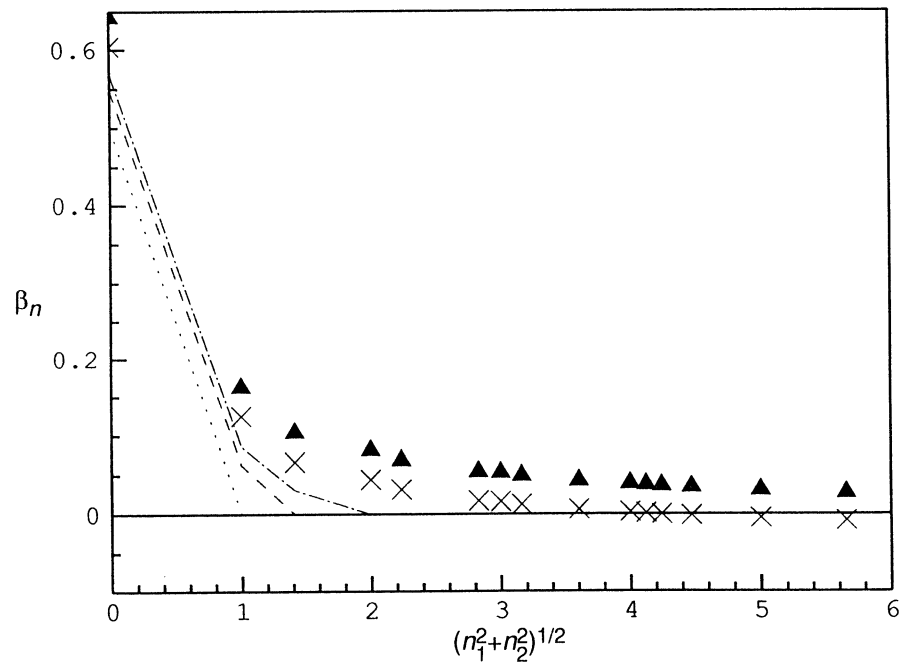

Fig. 2. Variational wavefunctions obtained by minimising equation (17) on a 16 × 16 lattice using 1 parameter (dotted line), 2 parameters (dashed line) and 3 parameters (dash–dot line). The exact ground state wavefunctions on a 16 × 16 (crosses) and infinite (triangles) lattice are also shown.

4. Conclusions

We have examined the accuracy of the method of variational wavefunctions in Hamiltonian lattice gauge theory for a case for which the exact ground state can be found analytically, namely non-compact U(1) gauge theory in (2+1) dimensions. The method was applied to moderate-sized lattices (8×8 and 16×16) using trial wavefunctions with up to 4 parameters.

We found that estimates obtained for the ground state wavefunction were, to a good approximation, independent of the lattice size for lattices large compared to the plaquette correlations implicit in the trial wavefunctions. For instance, the 3-parameter trial wavefunction incorporating self-correlation, nearest-neighbour plaquette correlations and diagonal-neighbour correlations, gave estimates of the ground state which were almost identical for both lattice sizes. Furthermore, the wavefunction obtained agreed very well with the exact result for the smaller lattice, but not for the larger lattice. As a rule of thumb, we would suggest that trial wavefunctions should include correlations up to at least one quarter the spatial extent of the lattice. For a 16×16 lattice this would require a trial wavefunction with 9 or 10 parameters.

A notable peculiarity of the exact ground state of the model considered in this paper is the presence of a δ-function factor restricting the sum of plaquette variables to be zero. It is not clear if this factor is unique to non-compact free U(1) theory, or whether it is also relevant to less trivial theories such as compact U(1), non-Abelian theories or theories with fermions. In any case, our numerical calculations indicate that the ground state wavefunction is well approximated in the model considered if one ignores this factor in the trial wavefunction. Since the bulk of computing time is expended in scanning the parameter space to locate the point which minimises the expectation value of the Hamiltonian, ignoring the δ-function represents a significant saving. Once the point is located, we found that introducing a cutoff on the accepted Monte Carlo sweeps to model the δ-function further improved the estimate of the ground state energy. We suspect this may also be true of other expectation values.

Finally, we remark that, although the method was able to estimate the exact 8×8 lattice ground state very well with modest computing time and facilities, we expect the amount of computing time required in general to rise rapidly with lattice size. The problems associated with adding the extra parameters needed for trial wavefunctions on larger lattices are twofold. Firstly, the scanning process to locate the minimum energy in a higher-dimensional parameter space is more complicated, and secondly, each Monte Carlo update becomes more time-consuming as new plaquette correlations are included. Neither of these problems has a counterpart in the standard Euclidean path integral simulations, where the one-plaquette action suffices irrespective of lattice size. We therefore foresee disadvantages for this method, compared with Euclidean Monte Carlo lattice gauge theory, when applied to large lattices.

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