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Systematic lower bounds for lattice Hamiltonians

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Abstract. The variational version of the Weinstein-Aronszajn method, for constructing sequences of intermediate Hamiltonians with spectra converging to the exact eigenvalues from below, is revived for lattice theories. A first test is performed on the critical Ising quantum chain and U(1)-invariant gauge systems. Special emphasis is put on applications to degenerate levels. A related upper bound construction is also discussed.

1. Introduction

In Hamiltonian formulation, the solution of lattice field theories is still in its exploratory phase. Most of the effort is spent on accurate characterisation of the ground state. This question is of considerable interest in statistical physics problems such as the existence of the antiferromagnetic order and its role in high temperature superconductivity. In quantum field theories one is mainly interested in the excitation spectrum.

Two types of systematic approach have been applied in this context so far. Various versions of the Hamiltonian Monte Carlo method (Kalos 1962, Chin *et al* 1985, Heys and Stump 1983, Barnes *et al* 1986) should yield accurate eigenvalues and eigenvectors, when statistical errors are reduced. Among the numerous non-stochastic methods the popularity of the Lánczos algorithm is growing (Irving 1985). Its iterated application (Alberty *et al* 1984, Dagotto and Moreo 1985) to states having non-zero overlaps with the exact levels yields systematic upper bounds for each level of the spectra.

The main difficulty with the Hamiltonian strategy is the explosively increasing number of states when, for instance, weak coupling calculations are performed in a strong coupling basis.

To cure this shortcoming, in stochastic methods *importance sampling* techniques are applied with the help of trial (variational) ground-state functionals forcing the random walk in the Hilbert space to its most significant part.

Various proposals for the effective truncation of the state space have been tested for the Lánczos method too (Patkós and Ruján 1985). Another direction of research is the variational generalisation of the Lánczos method (Duncan and Roskies 1985). In the latter case the application of weak coupling bases to lattice calculations has also been attempted.

The purpose of the present paper is to investigate the potential applicability of another systematic approach for finding *lower* bounds to the spectra. This non-stochastic algorithm eventually converges to the exact values. The algorithm has been known for quite some time, having grown out from the results of Weinstein (1935). (For reviews see Fox and Rheinboldt (1966) and Abdel-Raouf (1982).) The present

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form which is called a 'sequence of intermediate problems of second type' was proposed by Aronszajn in the early 1950s. Its application to quantum theory apparently stopped at the lithium atom (Reid 1974).

The main technical interest of the method is that at each intermediate stage the eigenvalue problem is reduced to a finite Hilbert space.

One constructs an infinite sequence of so-called intermediate problems:

$$H^{(k)} = H^{(0)} + B^{(k)} \tag{1.1}$$

starting with an almost arbitrary split of the original Hamiltonian into two parts

$$H = H^{(0)} + B \tag{1.2}$$

where B should be a positive operator ($(u, Bu) > 0$). Exploiting the max-min principle and the monotonicity principle of Weyl (Fox and Rheinboldt 1966) one establishes the inequalities

$$\lambda_l^{(k)} \leqslant \lambda_l^{(k+1)} \qquad \lim_{k\to\infty} \lambda_l^{(k)} \to \lambda_l(\text{exact}). \tag{1.3}$$

The index (k) is called the order of the approximation and practically equals the number of *energy layers* of $H^{(0)}$ where $H^{(k)}$ acts non-trivially (in a layer one might have several degenerate levels) while leaving in the complement of this subspace all the levels of $H^{(0)}$ intact. If $H^{(0)}$ coincides with the strong coupling Hamiltonian, the extension of the Hilbert space of $H^{(k)}$ to $H^{(k+1)}$ follows the E-scheme proposed by Hamer and Irving (1983).

In § 2 we describe the most important features of the proposed method (which might be called the Weinstein–Aronszajn construction) using the evergreen example of the transverse Ising model for illustration. Some practical questions, related to applications to degenerate levels, which are not easily accessible in the mathematical literature are discussed in appendix 1.

Section 3 presents the results from applying the method to simple gauge-invariant systems. In particular, we took the example of a U(1)-symmetric chain of plaquettes studied recently by Barnes and Kotchan (1987) with stochastic Hamiltonian techniques. The accuracy of our estimates compares very favourably already at low orders to their guided random walk (GRW) counterparts. We point out the existence of some temporary numerical instabilities, which disappear when the calculations are pushed to sufficiently high order. The other gauge-invariant Hamiltonian studied below is that of a 2×2 U(1)-symmetric plaquette system. The application of the proposed technique to systems of actual physical interest is under investigation.

In order to reduce the number of variables as much as possible, we use Hamiltonians with maximal spatial gauge fixing. The explicit form of such a Hamiltonian is constructed in appendix 2.

2. The intermediate problems of Weinstein and Aronszajn

The construction is reviewed below through the example of the exactly solved Ising quantum chain:

$$H = -\sum_{n=1}^{N} \sigma_n^z - x \sum_{n=1}^{N} \sigma_n^x \sigma_{n+1}^x. \tag{2.1}$$

Its splitting into the form (1.2) is defined as

$$H^{(0)} = -\sum_{n=1}^{N} \sigma_n^z - x\alpha \qquad B = x\left(\alpha - \sum_{n=1}^{N} \sigma_n^x \sigma_{n+1}^x\right) \qquad \alpha > N \tag{2.2}$$

where σ^z, σ^x are Pauli matrices.

The construction of the intermediate Hamiltonian $M^{(k)}$ starts with computing the $k \times k$ matrix

$$M_{mn} = \langle u_n | B^{-1} | u_m \rangle \qquad m, n = 1, \ldots, k \tag{2.3}$$

where $|u_n\rangle$ usually are chosen to be the lowest k eigenvectors of $H^{(0)}$:

$$H^{(0)}|u_n\rangle = \lambda_n^{(0)}|u_n\rangle \tag{2.4}$$

(this is called the special choice of Bazley). For the moment we assume that all levels are non-degenerate; therefore each energy layer consists of a single level.

The operator

$$H^{(k)} = H^{(0)} + \sum_{m,n=1}^{k} M_{mn}^{-1} |u_n\rangle\langle u_m| \tag{2.5}$$

acts non-trivially in the k-dimensional subspace $\{|u_m\rangle\}_1^k$. (M_{mn}^{-1} denotes the inverse of the $k \times k$ matrix M_{mn}.) The higher eigenvalues coincide with those of $H^{(0)}$. (In the original literature they are called *persistent*.) The eigenvalue sequences of the subsequent $H^{(k)}$ operators obey the relations (1.3).

Matrix elements of B^{-1} were computed with help of the integral representation

$$B^{-1} = \int_0^\infty \mathrm{d}z\, \mathrm{e}^{-zB} = \int_0^\infty \mathrm{d}z\, \mathrm{e}^{-z\alpha} \prod_{i=1}^{N} (\cosh z + \sinh z \sigma_i^x \sigma_{i+1}^x). \tag{2.6}$$

The translationally invariant subspace has been investigated both in the sectors even and odd under spin reflection $\sigma^z \to -\sigma^z$. Then M_{mn} can be written as

$$M_{mn} = \sum_{t=0}^{[N/2]} \kappa_{mn}^t I_t$$

$$I_t = \int_0^\infty \mathrm{d}z\, \mathrm{e}^{-z\alpha}[(\cosh z)^{N-t}(\sinh z)^t + (\sinh z)^{N-t}(\cosh z)^t] \tag{2.7}$$

where the integers κ_{mn}^t were found with a computer program.

The variation of α offers the possibility for optimising the estimate. The optimal choice can be best explained in a graphic way. In figure 1(a) the eigenvalues of $H^{(0)}$ are depicted as functions of α. In the $k = 1$ approximation only the lowest level $\lambda_1^{(0)}(\alpha)$ is replaced by a new estimator $\lambda_1^{(1)}(\alpha)$. This estimate can be shown easily to increase monotonically (appendix 1). The new level scheme is displayed in figure 1(b). It is self-evident that α_{opt} is located at the crossing of the curves $\lambda_1^{(1)}(\alpha)$ and $\lambda_2^{(0)}(\alpha)$. In the kth-order intermediate problem the best ground-state estimate comes from the crossing of the $\lambda_1^{(k)}(\alpha)$ and $\lambda_{k+1}^{(0)}(\alpha)$ curves.

In field-theoretic models most eigenstates of $H^{(0)}$ are degenerate. Next, we extend the above analysis to degenerate spectra.

Assume that $\lambda_2^{(0)}(\alpha)$ is g-fold degenerate above the unique $\lambda_1^{(0)}(\alpha)$ level. We wish to find α_{opt} for $\lambda_1^{(l)}(\alpha)$, when $l < g + 1$. This last condition means that the degenerate subspace is only partially incorporated into the Weinstein-Aronszajn construction.

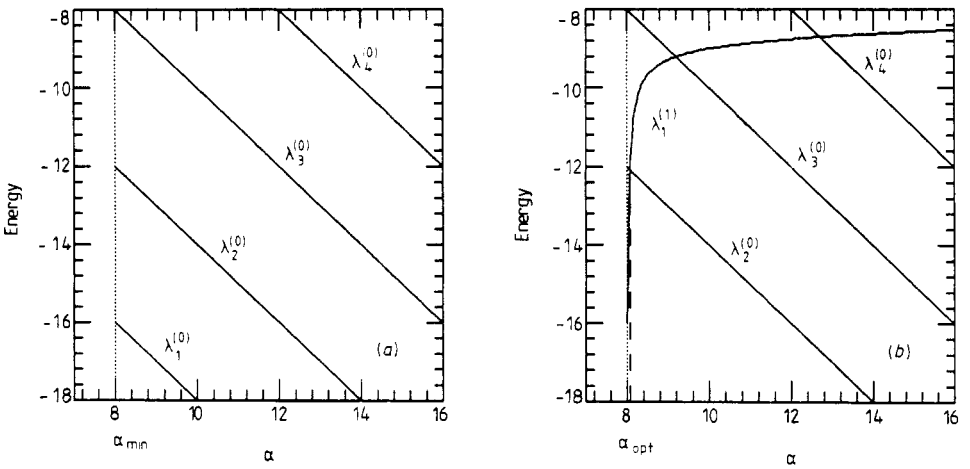

Figure 1. (*a*) Eigenlevels of (*a*) $H^{(0)}(\alpha)$ and (*b*) of the first intermediate problem as a function of the variational parameter α.

In appendix 1 we show that the function $\lambda_1^{(l)}(\alpha)$ takes invariantly the same value for $\alpha = \alpha_{\text{opt}}^{(1)}$ until $l < g+1$. As for $l < g+1$ there is at least one level of the degenerate layer $\lambda_2^{(0)}(\alpha)$ which is still persistent; the crossing point which determines $\alpha_{\text{opt}}^{(l)}$ remains the same. Only for $l = g+1$, when the layer $\lambda_2^{(0)}(\alpha)$ is exhausted, is $\alpha_{\text{opt}}^{(g+1)}$ pushed to larger values as it is determined by the crossing of $\lambda_1^{(g+1)}(\alpha)$ and $\lambda_3^{(0)}(\alpha)$. The above phenomenon is easily generalised to higher-lying degenerate levels, as illustrated in figure 2, where the subsequent ground-state energy estimates are displayed, as the tenfold degenerate $\lambda_3^{(0)}$ layer of the $N = 8$ Ising chain is gradually included into the Weinstein–Aronszajn construction.

For this reason in our tables below, we refer to the serial number of the energy layers and not of the levels of $H^{(0)}$ as the order of the approximation. This natural

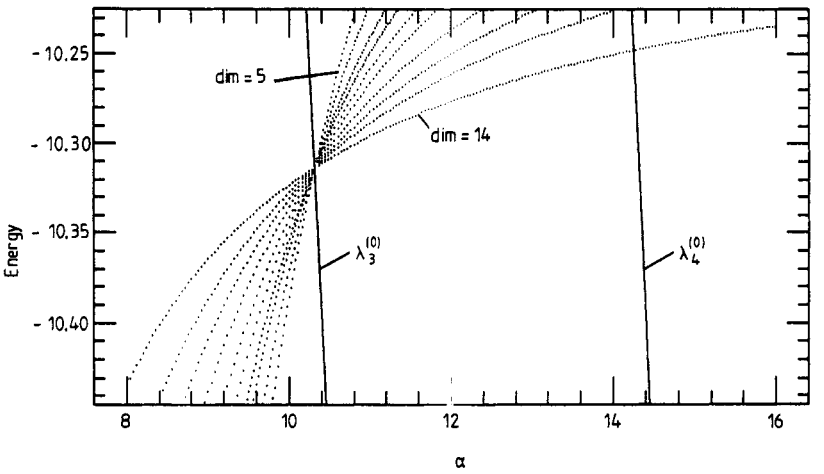

Figure 2. Evolution of the ground-state energy estimate when a degenerate energy layer is gradually included into the intermediate problem. Dotted curves display subsequent ground-state estimates and full lines indicate the untouched $H^{(0)}$ levels as a function of α.

organisation of the $H^{(0)}$ spectrum has been used earlier in the truncation of the strong coupling basis and is called the E-scheme by Hamer and Irving (1983).

We illustrate the accuracy of the method on the example of the critical Ising model ($x = 1$ in equation (2.1)). Table 1 shows the evolution of the ground-state energy in the first three orders for chains of size $N = 8$, 9, 10 and 12. Also given are the $\alpha_{\text{opt}}^{(3)}$ values and the known exact λ_1 eigenvalues.

We conclude this section with three remarks. Finite-size corrections to the energy density of two-dimensional infinite systems at the critical coupling are fully determined by their conformal characterisation (Blöte *et al* 1986, Affleck 1986). In figure 3 the correction for periodic chains computed with the present technique is compared with the theoretical prediction. The agreement is quite remarkable. Nevertheless, on a finer scale the deviation for $N = 10$–12 can be clearly seen even at third order.

Another practical observation might be that the variational parameter α can be optimised independently for each level. The lower half of table 1 presents estimates

Table 1. The ground-state energy of the Ising quantum chain from Weinstein's method as a function of size N. (The meaning of the different entries is explained in the text.)

N	$\lambda_1^{(1)}$	$\lambda_1^{(2)}$	$\lambda_1^{(3)}$	$\alpha_{\text{opt}}^{(3)}$	λ_1^{exact}
8	−12.07	−10.31	−10.252 04	14.252 04	−10.251 66
9	−14.03	−11.66	−11.519 49	14.519 49	−11.517 54
10	−16.01	−13.08	−12.791 01	14.791 01	−12.784 90
12	−20.00	−16.33	−15.354 41	15.354 41	−15.322 59
N			$\lambda_2^{(3)}$	$\alpha_{\text{opt}}^{(3)}$	λ_2^{exact}
8			−8.691 51	12.691 51	−8.690 94
9			−10.131 22	13.131 22	−10.128 36
10			−11.542 07	13.542 07	−11.533 43
12			−14.319 99	14.319 99	−14.278 39

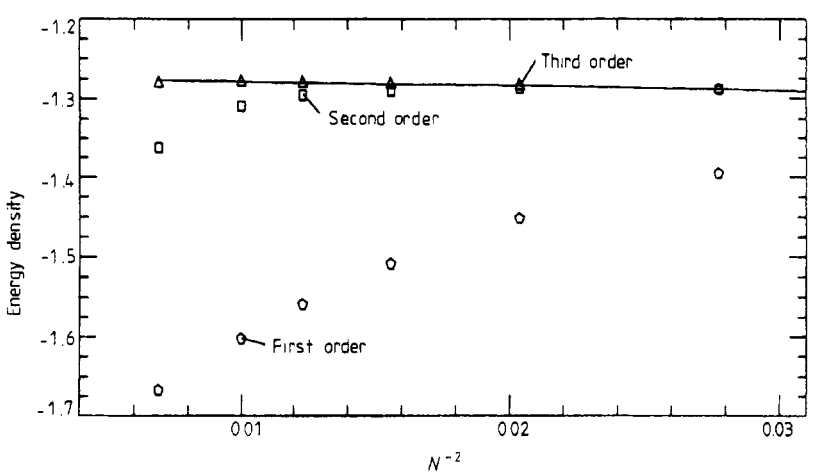

Figure 3. Conformal correction to the ground-state energy of the critical Ising chain. The full line is the theoretical prediction and the data points are the estimates given by the present numerical algorithm, improving with increasing order of approximation.

for the first excited state in the zero-momentum sector, even under spin reflection of the $N = 8, 9, 10, 12$ size chains.

Following Bazley (1961) one can also find upper bounds for the spectra, using the Weinstein-Aronszajn algorithm.

Consider the following splitting of the Ising Hamiltonian:

$$H = H^{(0)} - B \qquad H^{(0)} = -\sum_{n=1}^{N} \sigma_n^z + x\alpha \qquad B = x\left(\alpha + \sum_{n=1}^{N} \sigma_n^x \sigma_{n+1}^x\right) \tag{2.8}$$

where B is positive by $\alpha > N$. Repeating the usual procedure one defines a sequence of intermediate problems:

$$H^{(k)} = H^{(0)} - \sum_{m,n=1}^{k} M_{mn}^{-1} |u_n\rangle\langle u_m| \tag{2.9}$$

where B^{-1} is now the inverse of the B operator from (2.8). One easily finds that the $\lambda_i^{(k)}$ eigenvalues for each index i form descending series, converging eventually to the true ith eigenvalue of H from above. Simple calculation shows that

$$\mathrm{d}\lambda_i^{(k)}/\mathrm{d}\alpha \leqslant 0 \tag{2.10}$$

i.e., the optimal estimate arises when $\alpha \to \infty$. For the $N = 8$, 10 site long Ising chains this type of ground-state energy upper bounds were found from the third intermediate problem to be 1% accurate or better.

3. Application to U(1)-invariant gauge systems

The simplest gauge-invariant lattice system, which could test the proposed method is the U(1)-invariant periodic chain of plaquettes. Recently Barnes and Kotchan (1987) have obtained results for the ground state of this model using a guided random walk (RGW) algorithm.

The Hamiltonian of this system is easily obtained using appendix 2, because (A2.10) can be readily adapted to one-dimensional systems. The analogue of the constraint (A2.11) is absent, therefore in place of (A2.12) one finds:

$$H_{\mathrm{kin}} = \frac{1}{2\beta_t a_t} \sum_{x,y} \pi_p(x)\pi_p(y)[\delta_{x,y} - \tfrac{1}{4}(\delta_{x,y+1} + \delta_{x,y-1})]. \tag{3.1}$$

The splitting of the full Hamiltonian into the form (1.1) was chosen as

$$H^{(0)} = -\frac{1}{B_1} \sum_{p=1}^{N} \left(\frac{\partial^2}{\partial\Theta_p^2} - \frac{1}{2}\frac{\partial^2}{\partial\Theta_p\,\partial\Theta_{p+1}}\right) - B_2\alpha$$

$$B = -B_2\left(\sum_{p=1}^{N} \cos\Theta_p - N - \alpha\right) \tag{3.2}$$

where $B_1 \equiv 2\beta_t a_t$, $B_2 \equiv \beta_s / a_t$. In order to be able to compare our results directly with those of Barnes and Kotchan (1987) we set

$$B_1 = 2/\beta \qquad B_2 = \beta. \tag{3.3}$$

The intermediate problem is then worked out in the eigenvector set of $H^{(0)}$:

$$\psi(n_1, \ldots, n_N) = \exp\left(\mathrm{i}\sum_p n_p\Theta_p\right) \tag{3.4}$$

For the shortest chain ($N = 2$) we have performed the diagonalisation up to seventh order, where the dimension of the active subspace was 43. In table 2 the evolution of the estimates for the ground-state energy density ($E_0/2$) are given in the range $\beta = 1.0-4.0$ from fifth to seventh order. For comparison partly the GRW estimates are given, and partly the $o(\beta^{-1})$ weak coupling results derived also by Barnes and Kotchan (1987). It is notable that for $\beta = 2.5$ the result of the present investigation follows closely the weak coupling prediction, while the Monte Carlo simulation clearly overestimates it.

The empty entry at $\beta = 2.5$ in the fifth order of the approximation results from the instability of the corresponding intermediate problem in that range of α where the crossing should occur. In figure 4 the interval left out from the monotonically rising curve of the ground-state estimate can be characterised by the occurrence of a negative eigenvalue. This interval shifts away from the crossing region for higher-order approximations and the ground-state eigenvalue can be found with confidence.

Table 2. The ground-state energy of the U(1)-gauge symmetric plaquette chain as a function of β.

N	β	dim 31 order 5	dim 37 order 6	dim 43 order 7	GRW	SCE	WCE
2	0.5	0.468 882	0.468 883	0.468 883	0.470 ± 0.001	0.468 882	
	1.0	0.767 073	0.767 073	0.767 072	0.767 ± 0.003	0.766 927	0.835 447
	1.5	0.870 860	0.870 868	0.870 867	0.873 ± 0.006		0.882 020
	2.0	0.902 122	0.902 209	0.902 219	0.899 ± 0.009		0.904 151
	2.5		0.916 448	0.916 506	0.954 ± 0.015		0.917 060
	3.0	0.923 598	0.924 966	0.925 158			0.925 512
	3.5	0.927 373	0.930 495	0.930 957			0.931 473
	4.0	0.928 101	0.933 961	0.934 871			0.935 904
	4.5	0.926 121	0.935 752	0.937 310			0.939 325
		dim 1 order 1	dim 17 order 2	dim 33 order 3	GRW		
8	0.5	0.466 705	0.468 295	0.468 831	0.469 ± 0.000		

GRW: guided random walks.
SCE: strong coupling expansion.
WCE: weak coupling expansion.

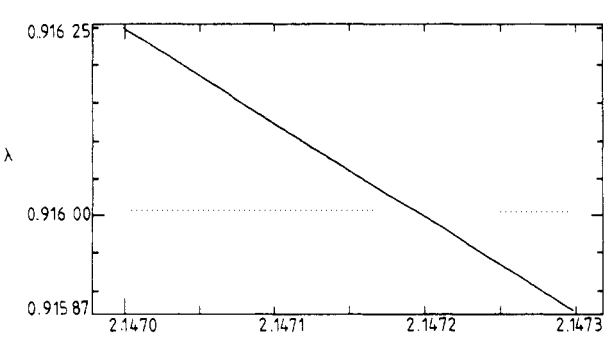

Figure 4. The instability of the ground-state energy estimator in the fifth order of the approximation ($N = 2$, U(1) gauge model). Along the suspended section of the dotted line a spurious negative eigenvalue of $H^{(5)}$ appears.

The last row of table 2 presents for illustrative purposes the energy density ($E_0/8$) of the $N=8$ system at $\beta=0.5$ in the first three orders of the approximation (33 states).

Another often-used test-system is the U(1)-symmetric quantum plane, the Hamiltonian version of the $(2+1)$-dimensional periodic QED. This system is fairly well understood on different levels of mathematical rigour (Polyakov 1977, Mack and Göpfert 1981). Here we report results for the smallest 2×2 plane. The Hamiltonian directly follows from (A2.13) and is given as

$$\begin{aligned} H_0 &= \tfrac{1}{2}\beta^{-1}[(\pi_1+\pi_2-\pi_3)^2+(\pi_1-\pi_2+\pi_3)^2+2(\pi_1-\pi_2-\pi_3)^2]-\beta\alpha \\ B &= \beta[\alpha-\cos\Theta_1-\cos\Theta_2-\cos\Theta_3-\cos(\Theta_1+\Theta_2+\Theta_3)] \end{aligned} \tag{3.5}$$

where $\beta_t a_t=\beta_s/a_t\equiv\beta$ and $\pi_1=-i\partial/\partial\Theta_l$ are understood. The construct has been performed up to fourth order. The degeneracies of the energy layers to this order are given as: 1, 12, 6, 24. No instability range of α was detected. The evolution of the ground-state energy in the range $\beta=0.5-2.0$ is shown in table 3. Towards the weak coupling ($\beta\to\infty$) regime the quality of the eigenvalue estimates deteriorates. At the same time the value of α_{opt} approaches quickly to the trivial value of $\alpha=4$. The last column of this table gives the upper bounds from the $k=4$ intermediate problem (2.9).

Table 3. The ground-state energy of the 2×2 U(1)-invariant plane system. The last column provides upper bounds based on equation (2.9).

β	dim 1 order 1	dim 13 order 2	dim 19 order 3	dim 43 order 4	dim 43 order 4
0.5	−0.130 693	−0.127 598	−0.127 151	−0.127 106	−0.12697
1.0	−2.0	−1.155 791	−1.086 867	−1.079 189	−1.0583
1.5	−4.66	−3.344 435	−2.954 468	−2.884 329	−2.7127
2.0	−7.0	−6.0	−5.122 953	−4.910 992	−4.3935

We conclude that the above exploratory studies demonstrate the competitivity of the Weinstein method with other Hamiltonian algorithms. In particular, simultaneous application with the related upper bound estimates (§ 2) gives a clear indication of the accuracy of the levels, obtained to a given order.

Different splitting of the Hamiltonian operator would be welcome for applications in the weak coupling regime. Also some other variant of the use of the variational parameter α might lead to considerable improvements.

Acknowledgment

The authors have been introduced to the Weinstein approximants by a lecture series of A Duncan. They are grateful to him for many helpful discussions and participation in the early stages of the present investigation.

Appendix 1

In order to have simpler formulae we work out specifically the *second-order* approximation where the unique ground state and a g-fold degenerate excited level are assumed

to be present in $H^{(0)}$. The first improved eigenvalue estimate is obtained from the one-dimensional intermediate problem

$$H^{(1)}(\alpha) = H^{(0)} + \frac{1}{M_{11}} |u_1\rangle\langle u_1|. \tag{A1.1}$$

By simple algebra one finds the inequality

$$\frac{\mathrm{d}\lambda_1^{(1)}}{\mathrm{d}\alpha} = -1 + \frac{\langle u_1|B^{-2}|u_1\rangle}{(\langle u_1|B^{-1}|u_1\rangle)^2} \geqslant 0 \tag{A1.2}$$

which means the monotonic increase of $\lambda_1^{(1)}$ with α. The optimal estimate is determined by the equality

$$\lambda_1^{(1)}(\alpha_{\mathrm{opt}}) \equiv \left(\lambda_1^{(0)} + \frac{1}{M_{11}}\right)_{\alpha_{\mathrm{opt}}} = \lambda_2^{(0)}(\alpha_{\mathrm{opt}}). \tag{A1.3}$$

Next one proceeds to the intermediate problem incorporating $1 < l < g+1$ levels at $\alpha = \alpha_{\mathrm{opt}}$. The $g-l+1$ degenerate levels left outside the construction, at the present stage, take for $\alpha = \alpha_{\mathrm{opt}}$ still the same values. The modified levels are found from diagonalising:

$$H^{(l)} = \begin{pmatrix} \lambda_1^{(0)} + M_{11}^{-1} & M_{12}^{-1} & \cdots & M_{1l}^{-1} \\ M_{21}^{-1} & \lambda_2^{(0)} + M_{22}^{-1} & \cdots & M_{2l}^{-1} \\ \vdots & \vdots & \ddots & \vdots \\ M_{l1}^{-1} & M_{l2}^{-1} & \cdots & \lambda_2^{(0)} + M_{ll}^{-1} \end{pmatrix}. \tag{A1.4}$$

With help of (A1.3) one verifies easily that

$$\det|H^{(l)}(\alpha_{\mathrm{opt}}) - \lambda_2^{(0)}(\alpha_{\mathrm{opt}})I| = 0. \tag{A1.5}$$

This means that $\lambda_1^{(l)}(\alpha)$ crosses the lowest persistent eigenvalue again at $\alpha = \alpha_{\mathrm{opt}}$. Simple geometric consideration yields, taking into account the inequality (A1.2), that

$$\lambda_1^{(g+1)}(\alpha_{\mathrm{opt}}^{(g+1)}) > \lambda_1^{(g)}(\alpha_{\mathrm{opt}}) = \ldots = \lambda_1^{(1)}(\alpha_{\mathrm{opt}}). \tag{A1.6}$$

These results are easily extended to higher degenerate layers.

Appendix 2

The Hamilton operator of U(1)-symmetric gauge systems in $2+1$ dimensions will be derived with spatial gauge fixing. The procedure is that of Choe *et al* (1988).

One starts with the Euclidean action

$$-S = \sum_x \beta_s \cos(\Theta_1(x) + \Theta_2(x+\boldsymbol{e}_1) - \Theta_1(x+\boldsymbol{e}_2) - \Theta_2(x))$$

$$+ \sum_x \sum_{i=1,2} \beta_t \cos(\Theta_i(x) + \Theta_3(x+\boldsymbol{e}_i) - \Theta_i(x+\boldsymbol{e}_3) - \Theta_3(x)) \tag{A2.1}$$

where the Θ_i are angular variables. One evaluates the integrals over the time-like link variables $\Theta_3(x) \equiv \psi(x)$ taking the limit $\beta_t \to \infty$ in the action of the transfer operator:

$$
\begin{aligned}
(\hat{T}F)[\Theta_i(x+e_3)] &= \exp\Bigg(\beta_s \sum_x \cos[\Theta_1(x+e_3)+\Theta_2(x+e_1+e_3) \\
&\quad -\Theta_1(x+e_2+e_3)-\Theta_2(x+e_2)]\Bigg) \int_{-\pi}^{\pi} \prod_x \frac{\mathrm{d}\Theta_i(x)}{2\pi} \int_{-\pi}^{\pi} \prod_x \frac{\mathrm{d}\psi(x)}{2\pi} \\
&\quad \times \exp\Bigg(\beta_t \sum_x \sum_{e_i} \cos[\psi(x)-\psi(x+e_i)-\Delta\Theta_i(x)]\Bigg) F[\Theta_i(x)]. \qquad \text{(A2.2)}
\end{aligned}
$$

Here we have introduced $\Delta\Theta_i = \Theta_i(x+e_3)-\Theta_i(x)$, the variation of the variable $\Theta_i(x)$ between two time slices.

The integrals become simple Gaussians in the $\beta \to \infty$ limit. The result will be expressed in terms of the Fourier coefficients of $\Theta_l(x)$:

$$
\tilde{\Theta}_l(k) = \frac{1}{N} \sum_x \Theta_l(x) \exp\left(-\mathrm{i} \frac{2\pi}{N} kx\right) \qquad 0 \leq x_i \leq N-1 \qquad 0 \leq k_i \leq N-1. \qquad \text{(A2.3)}
$$

One introduces in the space of the four-dimensional vectors

$$
W(k) = \{\mathrm{Re}\,\Delta\tilde{\Theta}_1(k), \mathrm{Im}\,\Delta\tilde{\Theta}_1(k), \mathrm{Re}\,\Delta\tilde{\Theta}_2(k), \mathrm{Im}\,\Delta\tilde{\Theta}_2(k)\} \qquad \text{(A2.4)}
$$

a new set of basis vectors:

$$
\xi_1 = N^{-1/2}\begin{pmatrix} \cos 2\pi k_1/N - 1 \\ \sin 2\pi k_1/N \\ \cos 2\pi k_2/N - 1 \\ \sin 2\pi k_2/N \end{pmatrix} \qquad \xi_2 = N^{-1/2}\begin{pmatrix} -\sin 2\pi k_1/N \\ \cos 2\pi k_1/N - 1 \\ -\sin 2\pi k_2/N \\ \cos 2\pi k_2/N - 1 \end{pmatrix}
$$

$$
\xi_3(k) = N^{-1/2}\begin{pmatrix} -\cos \pi k_1/N \sin \pi k_2/N \\ -\sin \pi k_1/N \sin \pi k_2/N \\ \sin \pi k_1/N \cos \pi k_2/N \\ \sin \pi k_1/N \sin \pi k_2/N \end{pmatrix} \qquad \xi_4(k) = N^{-1/2}\begin{pmatrix} -\sin \pi k_1/N \sin \pi k_2/N \\ \cos \pi k_1/N \sin \pi k_2/N \\ \sin \pi k_1/N \sin \pi k_2/N \\ -\sin \pi k_1/N \cos \pi k_2/N \end{pmatrix} \qquad \text{(A2.5)}
$$

where $N = [\sin^2(\pi k_1/N) + \sin^2(\pi k_2/N)]$. Denoting $W\xi_i$ by $\bar{W}_i$, the result of the ψ integration takes the very simple form:

$$
\begin{aligned}
&\exp\Bigg\{\beta_s \sum_x \cos \Theta_P(x)\Bigg\} \int_{-\infty}^{\infty} \prod_{k_f}{}' \prod_{j=1}^{4} \mathrm{d}\bar{W}_i \int \prod_i^2 \mathrm{d}\tilde{\Theta}_i(k=0) \\
&\exp\Bigg(-\beta_t \sum_j \Delta\tilde{\Theta}_j(k)^2 - \beta_t \sum_{k_f}{}' \sum_{j=3}^{4} \bar{W}_j(k)^2\Bigg).
\end{aligned} \qquad \text{(A2.6)}
$$

The subscript k_f and the prime in the above formula refer to the independent k components ($\Theta^*(k) = \Theta(N-k)$) and also the integration over the $k=0$ components is separated.

The components $\bar{W}_1(k)$ and $\bar{W}_2(k)$ are missing from the kernel of (A2.6); therefore the convergence over these variables would not be ensured. This dictates the choice of the following gauge conditions:

$$
\bar{W}_1(k) = \bar{W}_2(k) = 0 \qquad k \in k_f \qquad k \neq 0. \qquad \text{(A2.7)}
$$

The dependence on the $\bar{W}_3$ and $\bar{W}_4$ variables can be re-expressed in simple terms when using the plaquette variables:

$$\Theta_p(x+\tfrac{1}{2}(e_1+e_2)) = \Theta_1(x)+\Theta_2(x+e_1)-\Theta_1(x+e_2)-\Theta_2(x). \tag{A2.8}$$

Using its Fourier expansion one finds

$$\exp\left(\beta_s \sum_{x_p} \cos\Theta_p(x_p)\right) \int_{-\infty}^{\infty} \prod_{k_f}{}' \, d\tilde{\Theta}_p(k) \int \prod_i^2 d\tilde{\Theta}_i(k=0)$$

$$\exp\left\{-\beta_t \sum_j \Delta\tilde{\Theta}_j(k=0)^2 - \beta_t \sum_{k_f}{}' N^2 |\Delta\tilde{\Theta}_p(k)|^2\right\} F[\Theta_p(x), \tilde{\Theta}_j(k=0)]. \tag{A2.9}$$

Here we assume that the wavefunctional depends only on gauge invariant variables.

It is obvious from (A2.9) that the $\tilde{\Theta}_j(k=0)$ variables follow free dynamics; therefore the lowest energy values of the system correspond to the unexcited state of these degrees of freedom. The non-trivial dynamics is expressed solely through plaquette variables.

Their effective classical Hamiltonian is given by

$$H_{\text{eff}} = \beta_t a_t \sum_{k_f}{}' N(k)^2 |\dot{\tilde{\Theta}}_p(k)|^2 - \frac{\beta_s}{a_t} \sum_{x_p} \cos\Theta_p(x_p) \tag{A2.10}$$

where the time derivative $\dot{\Theta}_p \approx \Delta\Theta_p / a_t$ is introduced and the time-continuum limit is defined by keeping $\beta_t a_t$ and β_s / a_t fixed.

The canonical quantisation of (A2.10) is subject to the constraint

$$\sum_{x_p} \Theta_p(x_p) = 0. \tag{A2.11}$$

This constraint is taken into account simply by expressing one arbitrarily chosen plaquette from it and substituting this expression into the formulae relating the independent $\tilde{\Theta}(k)$ variables to the independent $\Theta(x)$ variables.

The result of the standard procedure for the kinetic part of the Hamiltonian is slightly different for the N = even and N = odd cases:

$$H_{\text{kin}} = \frac{1}{2\beta_t a_t} \sum_{x,y}{}' \pi_p(x)\pi_p(y)$$

$$\{\delta_{x,y} - \tfrac{1}{4}[\delta_{x_1,y_1}(\delta_{x_2,y_2+1}+\delta_{x_2,y_2-1}) + \delta_{x_2,y_2}(\delta_{x_1,y_1+1}+\delta_{x_1,y_1-1})]\} \tag{A2.12}$$

if N = odd and

$$H_{\text{kin}} = H_{\text{kin}}(N=\text{odd})$$

$$-\frac{1}{4\beta_t a_t N^2}\left[2\left(\sum_x{}' \pi_p(x)(-1)^{x_1+x_2}\right)^2 + \left(\sum_x{}' \pi_p(x)(-1)^{x_1}\right)^2 + \left(\sum_x{}' \pi_p(x)(-1)^{x_2}\right)^2\right] \tag{A2.13}$$

if N = even. The difference vanishes when $N \to \infty$, but for very small systems it is important. For the $N = 2$ toy model discussed in the text, it gives a change of factor 2 in the kinetic term. The prime over the summations in (A2.12) and (A2.13) means that an arbitrarily chosen plaquette has been left out. The Hamilton operator is obtained by replacing the canonical momenta $\pi_p(x)$ by $-i\partial/\partial\Theta_p(x)$.

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