

## Improvement of the Monte Carlo Projector Method for Spin Systems\*

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A different implementation of the Monte Carlo projector method is presented. It is based upon parallel scoring and population tracking techniques. The algorithm was tested in the analysis of the quantum spin Potts model  $P(q)$  on a lattice of  $(1+1)$ -dimension. Comparison with other techniques shows an improved accuracy of the results. © 1988 Academic Press, Inc.

### 1. INTRODUCTION

The Monte Carlo projector method is a powerful tool which can be used successfully to perform numerical simulation of lattice models, especially spin models. However, the accuracy of the results obtained for different cases proves to depend largely upon the particular model considered and the technique used. Several variations of the basic algorithm [1] (usually called (NE + NT)/NE method) have been proposed to obtain better results. Among them there are two which demand special attention: The population tracking method [2] and the parallel scoring technique [3]. Applications to simple models [1-5] suggest that, in general, the first one is a procedure which tends to decrease fluctuations even when an adequate a priori knowledge of the Hamiltonian eigenstates is not available; while the second one, even useful to reduce systematic errors, in certain cases gives rise to large fluctuations unless the eigenstates are sufficiently well known. It would then be of interest to develop an algorithm with the features of both foregoing ones. We present here an algorithm pointing to that direction, which we shall call the population tracking-parallel scoring algorithm (PTPS), which is based on an appropriate combination of the population tracking and parallel scoring techniques, working complementarily. We should also mention that because the standard population method presents instabilities we have also introduced a modification of this method in order to cope with them.

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We have chosen the one-dimensional quantum spin Potts  $P(q)$  model in a transverse field to illustrate the features of our proposal. For  $q=2$  this model becomes the well-known quantum Ising model which has been studied before with the projector method in some particular cases [1–4]. These previous results were used for comparison. A description of the PTPS procedure is presented in Section 2. The model and the numerical results are placed in Section 3 and, finally, Section 4 contains our conclusions and some remarks.

## 2. THE METHOD

We shall present here a brief description of the projector method [3–5]. To this end consider first a hamiltonian  $H$  and let  $E_i$ ,  $|\psi_i\rangle$ ,  $i=0, 1, \dots$  be its eigenvalues and eigenvectors, respectively, choosing for definitness  $E_0 \leq E_1 \leq E_2, \dots$ , etc. Now, if  $|\phi\rangle$  and  $|\chi\rangle$  are two vectors of the Hilbert space spanned by  $\{|\psi_i\rangle\}$ , such that

$$\langle \phi | \psi_j \rangle = \langle \chi | \psi_j \rangle = 0 \quad \text{for all } j < i \text{ (} i \geq 0 \text{)} \quad (2.1a)$$

and

$$\langle \phi | \psi_i \rangle \neq 0, \quad \langle \chi | \psi_i \rangle \neq 0 \quad (2.1b)$$

then

$$e^{-\beta' E_i} = \lim_{\beta \rightarrow \infty} \frac{\langle \chi | e^{-(\beta + \beta')H} | \phi \rangle}{\langle \chi | e^{-\beta H} | \phi \rangle}. \quad (2.2)$$

Notice that only one of the equalities (2.1a) is necessary because the eigenstates  $|\psi_i\rangle$  are orthogonal.

The Monte Carlo projector method provides us an algorithm designed to evaluate the right-hand side of (2.2). The limit involved in this equation is computed by introducing a large integer  $N$  such that

$$\beta = N\tau; \quad \beta' = N \Delta\tau \quad (2.3)$$

so that one can write

$$e^{-N \Delta\tau E_i} = \frac{Z(N, \tau + \Delta\tau)}{Z(N, \tau)} = \frac{\langle \chi | e^{-N(\tau + \Delta\tau)H} | \phi \rangle}{\langle \chi | e^{-N\tau H} | \phi \rangle}. \quad (2.4)$$

Now one splits  $H$  as

$$H = H_1 + H_2, \quad (2.5)$$

according to some criteria that will be discussed below. After this splitting, and for small  $\tau$ ; we can make the approximation:

$$T(\tau) = e^{-\tau(H_1 + H_2)} \cong e^{-\tau H_1} e^{-\tau H_2} = T_1(\tau) T_2(\tau). \quad (2.6)$$

Therefore one has for the  $Z$  function

$$Z(N, \tau) = \langle \chi | [T_1(\tau) T_2(\tau)]^N | \phi \rangle. \quad (2.7)$$

The next step is to introduce a complete set of states  $\{|i\rangle\}$  between each factor of  $T_k$ . Then we have

$$\begin{aligned} Z(N, \tau) = & \sum_{\substack{i_1, i_2, \dots, i_{N+1} \\ j_1, j_2, \dots, j_N}} \langle \chi | i_{N+1} \rangle \langle i_{N+1} | T_1(\tau) | j_N \rangle \langle j_N | T_2(\tau) | i_N \rangle \dots \\ & \langle i_2 | T_1(\tau) | j_1 \rangle \langle j_1 | T_2(\tau) | i_1 \rangle \langle i_1 | \phi \rangle. \end{aligned} \quad (2.8)$$

In order to evaluate this expression it is convenient to define "probabilities" ( $P$ ) and "scores" ( $S$ ) in the following way:

$$\langle i | T_k(\tau) | j \rangle = S_{ij}^{(k)}(\tau) P_{ij}^{(k)}(\tau), \quad k = 1, 2 \quad (2.9a)$$

$$\langle i | \phi \rangle = p_i \phi_i. \quad (2.9b)$$

The probabilities should certainly verify

$$P_{ij}^{(k)}(\tau) \geq 0, \quad p_i \geq 0 \quad \text{for all } i, j; k = 1, 2 \quad (2.10a)$$

$$\sum_i P_{ij}^{(k)}(\tau) = \sum_i p_i = 1. \quad (2.10b)$$

Then (2.8) is equivalent to

$$Z(N, \tau) = \sum_{\alpha} S_{\alpha}(\tau) P_{\alpha}(\tau) \quad (2.11a)$$

with

$$\alpha = \alpha(i_1, j_1, i_2, j_2, \dots, i_N, j_N, i_{N+1}), \quad (2.11b)$$

$$S_{\alpha}(\tau) = \chi_{i_{N+1}} S_{i_{N+1} j_N}^{(1)}(\tau) \dots S_{i_2 j_1}^{(1)}(\tau) S_{j_1 i_1}^{(2)}(\tau) \phi_{i_1}, \quad (2.11c)$$

$$\chi_{i_{N+1}} = \langle \chi | i_{N+1} \rangle,$$

$$P_{\alpha}(\tau) = P_{i_{N+1} j_N}^{(1)}(\tau) \dots P_{i_2 j_1}^{(1)}(\tau) P_{j_1 i_1}^{(2)}(\tau) p_{i_1}. \quad (2.11d)$$

Equation (2.11a) gives  $Z(N, \tau)$  as the mean value of a random variable which takes the values  $S_{\alpha}(\tau)$  with probability  $P_{\alpha}(\tau)$ .

The projector algorithm generates a set of samples of  $S_{\alpha}(\tau)$ , each one with probability  $P_{\alpha}(\tau)$ , so that (2.11a) can be replaced by the arithmetic average of the samples.

To evaluate (2.4) one has to obtain samples of  $Z(N, \tau)$  and  $Z(N, \tau + \Delta\tau)$ . These seem to be two separate problems, but it is not the case. The parallel scoring technique [3] allows us to calculate  $Z(N, \tau)$  and  $Z(N, \tau + \Delta\tau)$  simultaneously. To do this, we consider a single set of probabilities  $P_{ij}^{(k)}$ , so that we have

$$\langle i | T_k(\tau) | j \rangle = S_{ij}^{(k)}(\tau) P_{ij}^{(k)}, \quad k = 1, 2 \quad (2.12a)$$

$$\langle i | T_k(\tau + \Delta\tau) | j \rangle = S_{ij}^{(k)}(\tau + \Delta\tau) P_{ij}^{(k)}, \quad k = 1, 2 \quad (2.12b)$$

instead of (2.9a). Therefore, one set of samples for  $S(\tau)$  and another one for  $S(\tau + \Delta\tau)$  can be evaluated by means of a single set of configurations.

Equation (2.12) does not define probabilities and scores unequivocally. Then, different probability distributions can be chosen in order to end with better results. We have used the standard projector method distribution [1], given by

$$P_{ij}^{(k)} = \frac{|\langle i | T_k(\tau) | j \rangle|}{\sum_i |\langle i | T_k(\tau) | j \rangle|}, \quad k = 1, 2 \quad (2.13a)$$

$$S_{ij}^{(k)}(\tau) = \frac{\langle i | T_k(\tau) | j \rangle}{P_{ij}^{(k)}} \quad (2.13b)$$

$$S_{ij}^{(k)}(\tau + \Delta\tau) = \frac{\langle i | T_k(\tau + \Delta\tau) | j \rangle}{P_{ij}^{(k)}} \quad (2.13c)$$

$$p_i = \frac{|\langle i | \phi \rangle|}{\sum_i |\langle i | \phi \rangle|} \quad (2.13d)$$

$$\sigma_i = \frac{\langle i | \phi \rangle}{p_i}. \quad (2.13e)$$

Notice that when the matrix elements  $\langle i | T | j \rangle$  are positive,  $S_{ij}^{(k)}(\tau)$  is independent of  $i$ . Similarly if  $\langle i | \phi \rangle > 0$  for every  $i$ ,  $\sigma_i$  is a constant.

The accuracy of the results obtained with the parallel scoring procedure depends largely upon  $|\chi\rangle$  and  $|\phi\rangle$ . Our experience shows us that in general no accurate results can be obtained if previous information about the eigenstates  $|\psi_i\rangle$ , like variational states is not available.

On the other hand, it is also known that the population method is a technique which in certain cases could provide good results without having a detailed knowledge of the eigenstates of the system [2-4]. These two facts prompted us to combine the population method with the parallel scoring technique in the PTPS algorithm which can be described as follows:

(i) Build up an initial population of  $L_0$  members, each one consisting of an element of the basis  $\{|i\rangle\}$  which we may also call "a configuration," plus two running scores (one for  $Z(N, \tau)$  and one for  $Z(N, \tau + \Delta\tau)$ ).

(ii) Apply  $T(\tau)$  and  $T(\tau + \Delta\tau)$  to all the members of the population, modifying the running scores and obtaining a partial score  $\mathcal{S}_{(\text{member})}$  for  $T(\tau)$ .

(iii) Evaluate normalized scores

$$\mathcal{S}'_{(\text{member})} = \frac{L_0 \mathcal{S}_{(\text{member})}}{\sum_{\text{population's members}} \mathcal{S}_{(\text{member})}} \quad (2.14a)$$

Such that

$$\sum_{\text{population's members}} \mathcal{S}'_{(\text{member})} = L_0 \quad (2.14b)$$

(iv) Evaluate, for all members of the population

$$\mathcal{S}'_{(\text{member})} = I' + r, \tag{2.15}$$

where  $I'$  is an integer and  $0 \leq r < 1$ . Choose  $I = I' + 1$  or  $I = I'$ , at random, with probability  $r$  and  $1 - r$ , respectively; and keep  $I$  copies of the member. Notice that if  $I = 0$ , the member must be deleted.

After this we have a population of  $L_1$  members. (2.14b) ensures that  $L_1$  will be close to  $L_0$ .

(v) Repeat  $N$  times steps (ii) to (iv), obtaining a population of  $L_i$  members after the  $i$ -step.

At the end of the entire process we have a population of  $L_N$  members, each one containing samples of  $S_z(\tau)$  and  $S_z(\tau + \Delta\tau)$  which are used to evaluate [2.4]. This final population is used as input of step (ii) and the procedure is repeated many times in order to obtain a large number of samples. In practice we discard the first samples in order to reach a stationary regime.

In the standard population tracking procedure [4] one normalizes the scores with a reference score previously evaluated. In our procedure, we exploit the arbitrariness of this reference score and choose (Eqs. (2.14)) the best value in order to obtain a more stable number of members.

### 3. THE QUANTUM SPIN POTTS MODEL

We apply the projector method to evaluate the lowest lying energy levels of the  $(1 + 1)$ -dimensional quantum spin Potts model  $P(q)$  in a transverse field. For  $q = 2$  this model becomes the well-known quantum Ising model and for that reason it can be used as a test case for the present algorithm.

The hamiltonian of the  $P(q)$  model is given by [5]:

$$H = - \sum_{i=1}^s N_i - h \sum_{i=1}^s \sum_{k=1}^{q-1} \Omega_i^k \Omega_{i+1}^{q-k}, \tag{3.1}$$

where  $s$  is the number of spins in the  $(1 + 1)$ -dimensional lattice,  $N_i$  and  $\Omega_i$  are  $q \times q$  matrices given by

$$N_i = \begin{pmatrix} 0 & 1 & 1 & \dots & 1 & 1 \\ 1 & 0 & 1 & \dots & 1 & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & 1 & 1 & \dots & 0 & 1 \\ 1 & 1 & 1 & \dots & 1 & 0 \end{pmatrix} \tag{3.2a}$$

$$\Omega_i = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & \omega & 0 & \dots & 0 \\ 0 & 0 & \omega^2 & \dots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \dots & \omega^{q-1} \end{pmatrix}; \quad \omega = e^{2\pi i/q}. \quad (3.2b)$$

The periodic boundary conditions imply that

$$\Omega_{s+1} \equiv \Omega_1. \quad (3.3)$$

The corresponding vectors of the Hilbert space can be written in the form

$$|i\rangle = |i^1\rangle \otimes |i^2\rangle \otimes \dots \otimes |i^s\rangle, \quad (3.4)$$

where each  $|i^a\rangle$  is one of the  $q$  different states of the spin  $i$ .

Our purpose is to evaluate the two lowest energy levels,  $E_0$  and  $E_1$ , or equivalently the ground state  $E_0$  and the energy gap  $\Delta = E_1 - E_0$ . If we want to calculate  $E_1$  using (2.2) with the conditions (2.1), we must choose a vector  $|\phi\rangle$  such that  $\langle\psi_0|\phi\rangle = 0$  and  $\langle\psi_1|\phi\rangle \neq 0$ . Such a vector can be constructed with the help of a symmetry operator  $\Sigma$  capable of easily labeling the subspaces containing  $|\psi_0\rangle$  and  $|\psi_1\rangle$ . This operator exists and can be defined as

$$\Sigma = \prod_{i=1}^s \sigma^i = \prod_{i=1}^s \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 1 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & \dots & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 \end{pmatrix} \quad (3.5)$$

$\Sigma$  commutes with  $H$  and with all the  $N_i$ 's. Furthermore, it is easy to see that

$$\Sigma |\psi_0\rangle = |\psi_0\rangle. \quad (3.6)$$

The degeneracy of the first excited state does not allow the assignment of a definite value of the  $\Sigma$  operator in the  $q > 2$  case. In other words, there are vectors  $|\psi_1^{(+)}\rangle$  and  $|\psi_1^{(-)}\rangle$  both belonging to the eigenspace of  $E_1$ , which verify

$$\Sigma |\psi_1^{(+)}\rangle = |\psi_1^{(+)}\rangle \quad \text{and} \quad \Sigma |\psi_1^{(-)}\rangle = -|\psi_1^{(-)}\rangle. \quad (3.7)$$

If we choose a vector  $|\phi\rangle$  such that  $\Sigma |\phi\rangle = -|\phi\rangle$ , then (3.6) ensures that  $\langle\phi|\psi_0\rangle = 0$  and so we can obtain  $E_1$  from (2.2) using this vector.

It is worthwhile to notice that  $\Sigma$  reduces to the symmetry operator introduced by Kung *et al.* [4] for  $q=2$ .

### Implementation of the Projector Method

Now we apply the procedure of Section 2 to the present model. First we split the hamiltonian into the form

$$H = H_1 + H_2 = \sum_{i=1}^{R_1} \hbar_{2i-1,2i} + \sum_{i=1}^{R_2} \hbar_{2i,2i+1}, \quad (3.8a)$$

where

$$R_1 = \left[ \frac{s+1}{2} \right], \quad R_2 = \left[ \frac{s}{2} \right]$$

([ ] means integer part of), and

$$\hbar_{ij} = -N_i - h \sum_{k=1}^{q-1} \Omega_i^k \Omega_j^{q-k}. \quad (3.8b)$$

With this splitting of the hamiltonian into odd ( $H_1$ ) and even ( $H_2$ ) parts, already applied to the  $q=2$  case [4] and to models with fermions [5, 7, 8], we can set up the PTPS method in the form of a local iterative algorithm. It is evident that the terms in  $H_1$  (and in  $H_2$ ) commute; for this reason we can write

$$T_1(\tau) = \prod_{i=1}^{R_1} t_{2i-1,2i}(\tau); \quad T_2(\tau) = \prod_{i=1}^{R_2} t_{2i,2i+1}(\tau) \quad (3.9a)$$

$$t_{ij}(\tau) = \exp(-\tau \hbar_{ij}). \quad (3.9b)$$

Then, the matrix elements of Eq. (2.12) can be split into products of partial quantities involving pairs of neighbour spins. Therefore, the evaluation of probabilities and scores requires the calculation of the matrix elements:

$$M_{ij}(\tau) = \langle i^1 i^2 | t_{12}(\tau) | j^1 j^2 \rangle. \quad (3.10)$$

Now, the probabilities and scores (2.12) can be written as

$$P_{ij}^{(k)} = \prod_{i=1}^{R_k} p_{2i+k-2,2i+k-1}; \quad k=1, 2 \quad (3.11a)$$

$$S_{ij}^{(k)}(\tau) = \prod_{i=1}^{R_k} \sigma_{2i+k-2,2i+k-1}(\tau) \quad (3.12b)$$

and, taking into account (2.13), we have

$$p_{ij} = \frac{|M_{ij}(\tau)|}{\sum_k |M_{kj}(\tau)|} \quad (3.12a)$$

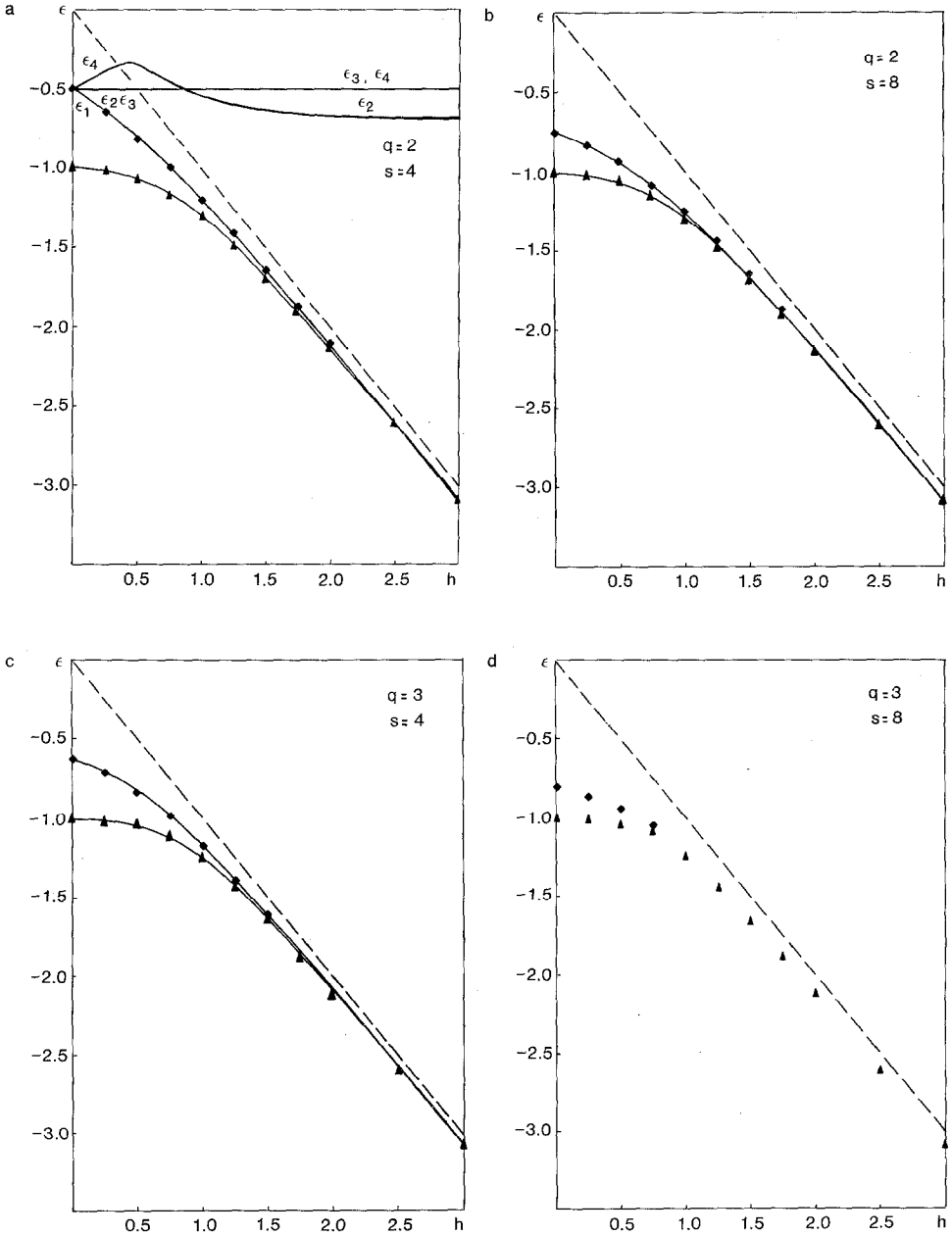


FIG. 1. Normalized energy levels versus  $h$  for several selected cases. The triangles correspond to  $\epsilon_0$  and the squares to  $\epsilon_1$ . Error bars (two standard deviations at each side) are smaller than the symbols. For clarity, the values for  $\epsilon_1$  were not included when superposition with the corresponding ones for  $\epsilon_0$  takes place. The full lines represent the exact results and the dashed ones show the asymptotic limit of  $\epsilon_0$  for  $h \rightarrow \infty$ .



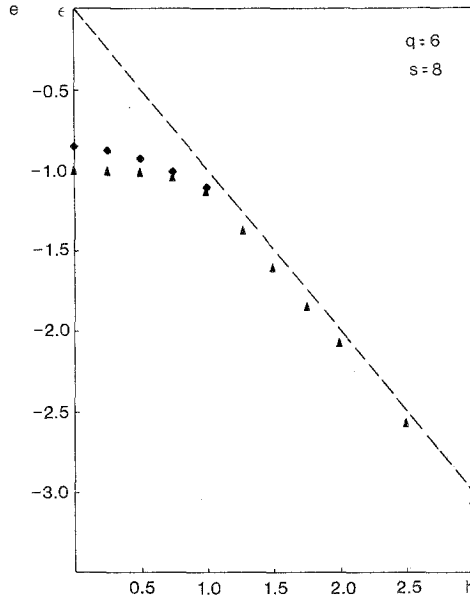


FIG. 1—Continued.

$$\sigma_{ij}(\tau) = \frac{M_{ij}(\tau)}{p_{ij}} \quad (3.12b)$$

$$\sigma_{ij}(\tau + \Delta\tau) = \frac{M_{ij}(\tau + \Delta\tau)}{p_{ij}}. \quad (3.12c)$$

In order to evaluate  $E_1$ , we should work in the representation where  $\sigma$  and  $N$  are diagonal. However, numerical calculations are simpler in the basis where  $\Omega$  is diagonal. If we call  $\tilde{M}$  the matrix obtained in this basis, then the matrix  $M$  (in the basis where  $\sigma$  and  $N$  are diagonal) is easily obtained by a similarity transformation

$$M = u^{-1} \tilde{M} u. \quad (3.13)$$

Some details of the calculations of  $\tilde{M}$  are given in the Appendix.

The ground state energy was evaluated working sometimes in one representation and sometimes in the other.

### Numerical Results

One of the purposes in our calculation, was to test the PTPS method in the detection of phase transitions in particular in the  $P(q)$  model. To this end we have computed the first two energy levels corresponding to the following cases:  $q=2$  to

6,  $s=4, 6, 8$ , and  $0 \leq h \leq 3$ . In our analysis it was convenient to define normalized energy levels as

$$\varepsilon_i = \frac{E_i}{(q-1)s}. \quad (3.14)$$

Then  $\varepsilon_0$  verifies

$$\varepsilon_0 = 1 \quad \text{for } h=0, \quad (3.15a)$$

$$\varepsilon_0 \sim -h \quad \text{for } h \rightarrow \infty \quad (3.15b)$$

for every  $q$  and  $s$ .

It is well known that the present model has, when  $s \rightarrow \infty$ , a phase transition at  $h=1$ , being of second order for  $q < 4$  and of first order otherwise [6]. The phases can be labeled by the degeneracy of the ground state, i.e., it is non-degenerated for  $h < 1$  and becomes degenerate for  $h \geq 1$ . The order of the transition is related to the continuity of the derivative of  $E_0$  with respect to  $h$ : In a first-order transition this derivative presents a discontinuity at the transition point.

In a finite system there are no such discontinuities and the ground state is non-degenerate for every  $h$ . However, the existence of a phase transition in the neighbourhood of  $h=1$  can be inferred from the vanishing tendency of the energy gap  $\Delta$ . The calculations were performed taking  $\beta=1.25$  and  $\Delta\tau/\tau=0.08$  in all the cases. About 100,000 samples of the energy levels were averaged at each point.

We present in Fig. 1 some representative examples of our results. When available, exact values of the energy levels were included for comparison. These exact values were obtained by direct numerical diagonalization of the hamiltonian of the corresponding finite system.

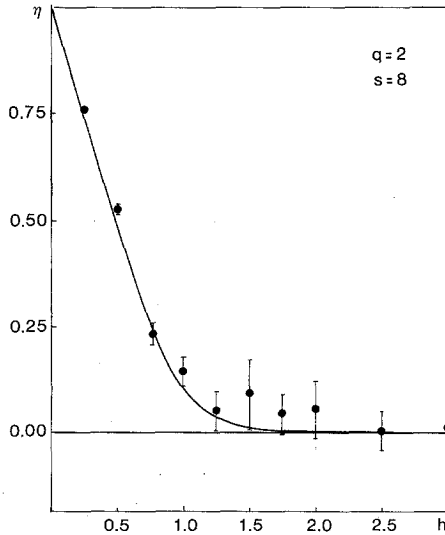


FIG. 2. Normalized energy gap  $\eta$  versus  $h$  for the particular case  $q=2, s=4$ . The full line corresponds to the exact result.

The vanishing tendency of the energy gap can clearly be seen, even in the smallest systems, confirming the appearance of a phase transition. However, an accurate determination of the value of the transition parameter  $h_c$  is not possible.

Figure 2 shows, for a particular case, the results for the normalized energy gap  $\eta = \Delta/q$ , provided by the PTPS method in contrast to the exact value.  $\eta$  was always computed by subtraction of the two first energy levels giving rise to greater errors. However, the calculated values are in good agreement with the exact ones.

Notice also that an alternative way of computing  $\eta$ , as the one proposed in Ref. [4], cannot be easily generalized for this model when  $q > 2$  and would imply a substantial increase of the computation time.

#### 4. CONCLUSIONS AND REMARKS

We want to start by making some remarks about our numerical calculations:

(i) The values of the different physical magnitudes should be independent of the basis  $\{|i\rangle\}$  used to perform calculations. In practice, however, numerical fluctuations could be different when working on a different basis. This is due to the fact that the probability distribution of the random variable whose mean is to be evaluated, does depend on the selected bases. Moreover, if the distribution is not sampled thoroughly enough, also the mean values may appear to depend on choice of basis. In order to analyze the dependence of the results upon the selected basis, we have evaluated the ground state energy  $E_0$  twice by using the  $M$  and  $\tilde{M}$  bases, respectively. We have not detected any important difference between the corresponding results. This kind of test should be done in every particular application, not only to detect instabilities of the numerical method but also to find a basis which minimizes fluctuations.

(ii) The relative fluctuations in the number of members of the populations were less than 15% in all the cases studied. This is an important reduction in comparison with the values of the standard population tracking technique, which we found to be, in certain cases, superior than 200%.

(iii) All the elements of the matrix  $\tilde{M}$  are positive, but it is not the case with the  $M$ 's. For this reason, fluctuations are larger when calculations are performed with  $M$ . However, the number of negative elements in  $M$  is small when compared with the matrix size, so special population techniques for negative matrix elements [8] were not necessary. The modifications performed in the population updating procedure played an important role at this point. Nevertheless, it would be interesting to adapt such techniques to the present algorithm and apply them to systems with negative matrix elements. Work is in progress in that direction.

(iv) Computer time restrictions turned impossible for us to obtain a large number of samples in all the calculated cases. We could observe in some particular examples that increasing statistics result in smaller error bars.

(v) Our PTPS results obtained for  $E_0$  and  $E_1$  are truly independent of the initial state  $|\phi\rangle$  used, in contrast with large dependences found in previous works [1, 3, 4] which did not use population techniques. However, in order to reduce the number of discarded samples a variational state of the form

$$|\phi\rangle = \prod_{i=1}^s \begin{pmatrix} \cos \theta \\ \alpha \sin \theta \\ \vdots \\ \alpha \sin \theta \end{pmatrix}; \quad \alpha = (q-1)^{-1/2} \quad (4.1)$$

was used in almost every case.

On the other hand, a broad final state like  $|\chi\rangle = \sum_i |i\rangle$  was always used. The inclusion of other final states could, in principle, improve the results [4].

(vi) Before developing the PTPS method, we tried the following ones [1, 4]: (NE + NT)/NE, modified projector and parallel scoring, in order to adjust parameters and to make comparisons. For these proofs we used the probability distribution

$$P_{ij}^{(k)} = \frac{|\langle i | T_k(\tau) | j \rangle|^v}{\sum_l |\langle l | T_k(\tau) | j \rangle|^v}, \quad k = 1, 2; \quad v > 0 \quad (4.3)$$

instead of (2.13a), with several values of  $v$ . We decided to keep  $v = 1$  because in the other cases the algorithm becomes more involved without significant improvement of the results. We also made a comparison with pre-existent calculations in order to illustrate the performance of the PTPS method. In Fig. 3 we have plotted the results

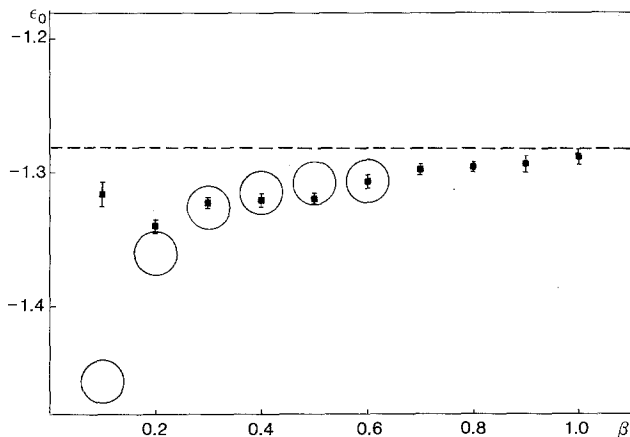


FIG. 3. Approximations to the ground state energy level  $E_0$  for the eight site  $q=2$  model, versus  $\beta$ . The dashed line corresponds to the exact value. The circles are a scaled reproduction of the black ones in Fig. 1 of Ref. 4. The squares are our PTPS results. When not drawn, error bars are smaller than the symbols.

obtained for  $E_0$  in the case of the eight site Ising model ( $q=2$ ). The big circles are a scaled reproduction of the black circles of Fig. 1 in Ref. [4] while the squares represent the PTPS result in similar conditions (broad final state) but without inclusion of information about the system eigenstates. Notice that the PTPS method is able to provide good results without the knowledge of the already mentioned a priori information about the eigenstates. It also implies a reduction of systematic errors (the succession of circles seems to converge very slowly to the exact value). The accuracy of the value obtained for  $\beta=0.1$  is accidental due to typical cancellations, very frequent when using parallel scoring.

(vii) Before starting the final calculations we tried several values of the parameters  $\beta$ ,  $\tau$ , and  $\Delta\tau$ . It was found that the selected values of these parameters are appropriate in the sense that no excessive truncation errors appear in the results.

We have presented a new implementation of the projector algorithm, based on two previous proposals [3, 4] and it has been applied to a particular case, the quantum Potts model. The analysis of its features has shown an actual improvement in the accuracy of numerical results when compared to previous ones. We have also shown that this method could be useful in the detection of phase transitions even if one is dealing with a very small number of sites.

We should also mention that all the numerical calculations presented in this work were done at the La Plata University Computer Center, in an IBM VM/370, CPU model 4361. In this machine, the evaluation of one energy level, for a given value of  $h$ , in an 8-spin system demands about 10 min of CPU time.

#### APPENDIX: CALCULATION OF $\tilde{M}$

From (3.9b) and (3.8b) we see that

$$t_{ij}(\tau) = \exp \left[ \tau N_i + \tau h \sum_{k=1}^{q-1} \Omega_i^k \Omega_j^{q-k} \right]. \quad (\text{A.1})$$

We take, with no loss of generality,  $i=1, j=2$ , and write

$$t(\tau) = t_{12}(\tau) = \exp \left[ \tau N + \tau h \sum_{k=1}^{q-1} \Omega_1^k \Omega_2^{q-k} \right]. \quad (\text{A.2})$$

Let

$$\theta = \sum_{k=1}^{q-1} \Omega_1^k \otimes \Omega_2^{q-k} \in \mathbb{R}^{q^2 \times q^2}. \quad (\text{A.3})$$

It is easy to see [9] that

$$\langle i^1 i^2 | \theta | j^1 j^2 \rangle = (q \delta_{i^1 i^2}^{(q)} - 1) \delta_{i^1 j^1} \delta_{i^2 j^2}, \quad (\text{A.4})$$

where  $\delta_{ij}^{(q)}$  is the standard Kronecker  $\delta$  modulo  $q$ :

The fact that  $\theta$  is a diagonal matrix can be used to avoid the evaluation of the exponential of a  $q^2 \times q^2$  matrix. If we define

$$\theta_1 = \begin{pmatrix} q-1 & 0 & \cdots & 0 \\ 0 & -1 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdots & -1 \end{pmatrix} \in \mathbb{R}^{q \times q} \quad (\text{A.5})$$

and

$$t'(\tau) = \exp(\tau N + \tau h \theta_1). \quad (\text{A.6})$$

Then it can be seen that

$$\tilde{M}_{ij}(\tau) = t'_{kl}(\tau) \delta_{i^2, j^2} \quad (\text{A.7a})$$

with

$$k = f(i^1, i^2, 1), \quad l = f(j^1, j^2, 1) \quad (\text{A.7b})$$

and

$$f(i, j, k) = \begin{cases} i & \text{if } i \neq j \text{ and } i \neq k \\ j & \text{if } i = k \\ k & \text{if } i = j. \end{cases} \quad (\text{A.8})$$

To evaluate  $t'(\tau)$  we use the well-known Trotter formula [10],

$$t'(\tau) = \lim_{n \rightarrow \infty} [t'_{1n}(\tau) t'_{2n}(\tau)]^n \quad (\text{A.9a})$$

with

$$t'_{1n}(\tau) = \exp\left(\frac{\tau}{n} N\right) \quad (\text{A.9b})$$

and

$$t'_{2n}(\tau) = \exp\left(\frac{\tau h}{n} \theta_1\right). \quad (\text{A.9c})$$

The evaluation of  $t'_{2n}(\tau)$  is trivial because  $\theta_1$  is diagonal. For  $t'_{1n}(\tau)$  we find that

$$t'_{1n}(\tau) = \alpha_{1n}(\tau) I + \alpha_{2n}(\tau) N \quad (\text{A.10a})$$

with

$$\alpha_{1n}(\tau) = \sum_{k=0}^{\infty} \frac{a_k}{k!} \left(\frac{\tau}{n}\right)^k, \quad \alpha_{2n}(\tau) = \sum_{k=0}^{\infty} \frac{b_k}{k!} \left(\frac{\tau}{n}\right)^k \quad (\text{A.10b})$$

and

$$\begin{aligned} a_0 &= 1, & b_0 &= 0, \\ a_k &= (q-1)b_{k-1} \\ b_k &= a_{k-1} + (q-2)b_{k-1}. \end{aligned} \quad (\text{A.10c})$$

Now we can evaluate (A.9). For practical reasons it is convenient to define

$$t_n''(\tau) = t_{1n}'(\tau) t_{2n}'(\tau) - I \quad (\text{A.11})$$

and use this matrix, rather than  $t_{1n}'(\tau) t_{2n}'(\tau)$  in the iterations. Using this procedure, we have calculated  $t'(\tau)$  with a minimum of 12 significant figures.

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