MULTI-SPIN CODING OF THE MONTE CARLO SIMULATION OF THE THREE-STATE RANDOM POTTS MODEL AND THE BLOCK-SPIN TRANSFORMATION

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ABSTRACT

The multi-spin coding of the Monte Carlo simulation of the three-state Potts model on the simple cubic lattice is presented. The ferromagnetic (F) model, the antiferromagnetic (AF) model, and the random mixture of the F and AF couplings are treated. The multi-spin coding technique is also applied to the block-spin transformation. The block-spin transformation of the F Potts model is simply realized by the majority rule, whereas the AF three-state Potts model is transformed to the block spin having a six-fold symmetry.

1. Introduction

Monte Carlo simulations are used as standard techniques to investigate statistical mechanical properties of many-body systems. In treating large systems, especially near the critical points and at very low temperatures, we often encounter slow dynamics. To overcome such slow dynamics, the development of fast algorithms is demanded. To gather more information from a single simulation is another direction of effort for algorithmic improvement. The cluster-flip Monte Carlo method, the histogram method, and the multicanonical simulations are examples of the recent progress.

For the simulations of the Ising model, where only one bit is required for storing the information of a single spin, a computer word can store several spins. Based on this fact, the multi-spin coding technique has been successfully developed. Among them, the idea
of the coding by Bhanot et al. and its variations are especially useful. In these methods, just a single bit is assigned to each spin. Instead of storing spins at different sites in the same lattice in a word, as in the case of former realizations of the multi spin coding, Ising spins at the same site of several independent systems (of the same lattice structure) are stored in a word. The spins for 32 (64) systems are updated simultaneously in the case of 32-(64-) bit machine, with a single random-number sequence; for that to be achieved, all the operations are executed by logical commands. As a result, the computation time is reduced remarkably. One can simulate either systems with different parameters, for example, the temperature, the external field, etc., or systems under the same parameters with different random number sequences. Even for the latter purpose, one needs to generate only one random-number sequence. In the case of the simulations of random systems, one can simulate systems with different configurations in parallel. Since an average over a large number of random configurations should be taken, the multi-spin coding technique is particularly effective for random systems. We should note that the multi-spin coding has also been applied to the Monte Carlo simulations of the Ising model on quasicrystals.

The Monte Carlo renormalization group (MCRG) is a powerful tool to analyze critical phenomena. In MCRG method, one performs the block-spin transformations at each Monte Carlo sweep. The block-spin transformation makes a block spin from \( b^D \) original spins, with the scale factor \( b \). The present authors have successfully used the multi-spin coding to the block-spin transformation of the three-dimensional (3D) Ising model.

The idea of the multi-spin coding can also be applied to other models with discrete symmetries. The \( q \)-state Potts model is one example. The Potts model has various interesting properties. The order of the phase transitions of the ferromagnetic (F) Potts model depend on the dimensionality, \( D \), and the number of the state, \( q \). In 3D, the F Potts model shows a first-order transition, whereas the antiferromagnetic (AF) model shows a second-order transition. The random mixture of F and AF couplings gives rise to new problems: The rounding of first-order transition in weak ferromagnetic region is one of interesting problems; one may also ask the universality of critical exponents in this case. The Potts glass phase will be another problem of interest. The zero-temperature transition of the three-state Potts glass has been suggested in 3D.

In this paper, we present the multi-spin coding of the three-state Potts model on the simple cubic lattice. For the coupling, we consider both cases of the F and AF couplings. The random mixture of the F and AF couplings are also treated. We also present the realization of the block-spin transformation using multi-spin coding technique. The appropriate choice of the block-spin transformation is essential to extract the critical properties of the order parameter. We employ quite different block-spin transformations for the F Potts model and the AF Potts model: The block-spin transformation of the F model is simply realized by the majority rule, whereas the block spin of the AF three-state Potts model has the same symmetry as the six-clock model.

2. Multi-Spin Coding

We are concerned with the three-state Potts Model, whose Hamiltonian is given as

\[
\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \delta S_i S_j ,
\]

(1)
where each spin $S_i$ can take three states, 0, 1 and 2. Here a variable $J_{ij}$ may take either $+J$ or $-J$ generally. In the following, we consider only the nearest-neighbor interactions.

We employ the multi-spin coding algorithm, which was originally used for the Ising model. In contrast to the Ising model, two bits are required to represent a Potts spin; the three states, 0, 1 and 2, are represented by (00), (01), and (10) in binary-number representation. Therefore, we assign one word for the upper bit and another word for the lower bit, as is seen in the following. It should be noted that the calculation of the order parameter becomes quite simple in this two-word representation, because the number of 1 (2) spin is counted just by summing up the lower- (upper-) bit throughout the lattice.

To update a spin in one of the three states, one has to choose either of the rest two states as a trial state. This procedure is executed by the following code:

```c
iscoin=ira(la)
isnew0=iand(not(isold0),iscoin)

isnew1=not(ior(isold1,iscoin))
```

The old spin is represented by (isold1, isold0), with the former word representing the upper bit and the latter the lower bit, respectively. Here, `ira` is a random number, where each bit takes 0 or 1 with the probability of 1/2. Then, the trial state, also represented by two words, (isnew1, isnew0), is selected as one of the other two states with an equal probability for every case of the old states (00), (01), and (10).

In the Metropolis algorithm, one needs to count the local energy change due to the above trial flip of a picked single spin. The following code is for calculating the energy change (in unit of $J$) at a bond:

```c
neqold = ior(ieor(isold0,is0),ieor(isold1,is1))
neqnew = ior(ieor(isnew0,is0),ieor(isnew1,is1))
ide0 = iand(neqold,neqnew)
ide1 = not(neqnew)
```

Two words (is1, is0) represent the nearest-neighbor spin in concern. The energy change is also given by the binary-number representation in two words, ide1 and ide0. The above code is for F Potts model. For AF model, the last line should be modified as follows:

```c
ide1 = not(neqold)
```

And for the random-bond model, the same line should be read as

```c
ide1 = ior(iand(jbond,not(neqnew)),not(ior(jbond,neqold)))
```

where `jbond` should either be 1 for the ferromagnetic bond or 0 for the antiferromagnetic bond. Since the coordination number is six for the simple cubic lattice, the local energy change $W$ takes an integer value between $-6$ and 6 in units of $J$. Thus, four words are necessary to represent $W$ in the multi-spin coding. It should be compared to the Ising case, where three words are enough to represent the local energy change.

In using the random-number sequence, we apply the trick proposed by Michael, rather than the original one by Bhanot et al. That is, we use the precalculated table for the transition probability, $\min[1,e^{-\beta J W}]$; in the original algorithm, on the other hand, the transition probability table is updated dynamically. In case of using the precalculated table, a large table is required to ensure the accuracy in temperature; one can, however, use a very large table easily in computers these days, so that it is not considered as a
drawback. On the other hand, using a small table which is dynamically updated may cause an uncontrollable temperature fluctuation.

We use a dummy variable $X$, which takes the integer value from 0 to 6. We prepare the table so that the probability to get the value of $X$ is given by

$$
X(r) = \begin{cases} 
0, & \text{if } r > e^{-K} \\
1, & \text{if } e^{-K} > r > e^{-2K} \\
2, & \text{if } e^{-2K} > r > e^{-3K} \\
3, & \text{if } e^{-3K} > r > e^{-4K} \\
4, & \text{if } e^{-4K} > r > e^{-5K} \\
5, & \text{if } e^{-5K} > r > e^{-6K} \\
6, & \text{if } e^{-6K} > r,
\end{cases}
$$

where $K = \beta J$ and $r$ is a random number which uniformly takes the value between 0 and 1. Then, the rule of the spin update will be as follows: If $(-W) + X + 8$ is greater than 8, then the spin will be flipped.

It should be emphasized that the shuffling of the precalculated $X$-table is effective for simulating different samples with the same parameters by a single random-number sequence. The statistical dependence of random sequences in conjunction with the shuffling of the table has been recently discussed.

The FORTRAN code for the Metropolis method is given in Appendix, which is for the F Potts model. In our multi-spin coding, $X$ is represented by three words, $(jxtb2, jxtb1, jxtb0)$. We use the integer random number, $irb$, which takes the value between 0 and $nword-1$. The decrease in the local energy at the trial flip, $(-W) + 8$, is calculated to be $(isum3, isum2, isum1, isum0)$ in binary-number representation.

The spin update is executed by the logical commands; $iflip$ is the flag for the flip. The updated spin and the resultant energy difference are given by $isp0$ and $iengd$, respectively. With slight modifications, which are commented out with '*', we can also treat the AF model and the $\pm J$ model; the information of the configuration of $\pm J$ bonds should be included in $jbond$, which in general depends on the lattice point $la$. For the convenience of vectorization, we divide the lattice into two interpenetrating sublattices.

The linear size of the system is given by $nx$; the number of the spins on each sublattice is given by $nla2=nx**3/2$. The periodic boundary conditions are employed, and informations on the neighboring lattice points are provided in the tables, $jx$, $jyr$, $jyl$, $jzl$ and $j2l$.

3. Block-Spin Transformation

3.1. Ferromagnetic Order Parameter

For the three-state F Potts model, it is convenient to express the order parameter as a two-dimensional vector. Three states 0, 1, and 2 are expressed by the vectors directing $\pm 2\pi/3$ from each other as shown in the inset of Fig. 1. Let us consider the case of the block-spin transformation from eight spins; that is, the scale factor $b$ is 2. Possible vectors obtained by the vector sum of eight Potts spins are shown in Fig. 1. From each vector, we make a block spin which also takes three states as does the original Potts spin; we choose the Potts
state directing closest to the vector as the block-spin state. The rule for determination of the block spin is illustrated in Fig. 1, where the separation is shown with solid lines. At the border, the random number will be used to determine which state is to be chosen.

One would find that the block-spin transformation described above is, in fact, equivalent to the simple majority rule; in other words, the three-state Potts spin is mapped onto the three-state Potts spin by the majority rule transformation.

The essential part of the FORTRAN code for the block-spin transformation is given as follows:

```fortran
block-spin transformation
ferro 3-state Potts to 3-state Potts

non02x = ior(isumx0, isumx1)
nsumx2 = not(isumx2)
non02y = ior(isumy0, isumy1)
nsumy2 = not(isumy2)
j0 = iand(iand(isumx0, isumx1), isumy1)
j1 = iand(iand(isumy0, isumy1), isumx1)

iran = ir(la)
iranx = iand(isumx2, iran)
irany = iand(isumy2, not(iran))

is0 = iand(isumx2, iand(nsumy2, non02y))
is0 = ior(is0, isumx3)
is0 = ior(is0, iand(isumx2, non02x))
```

Fig. 1. Possible vectors obtained by the vector sum of eight F Potts spins.
Here, the sum of 0-bit of eight Potts spins is expressed by \((\text{isum}_x^3, \text{isum}_x^2, \text{isum}_x^1, \text{isum}_x^0)\). Similarly, the sum of 1-bit is given by \((\text{isum}_y^3, \text{isum}_y^2, \text{isum}_y^1, \text{isum}_y^0)\). Two words, \((\text{ibnew}_1, \text{ibnew}_0)\), gives the block spin. The random number \(\text{ir}\) is used for tie breaking at the border. To make the MCRG analysis of the F order parameter, we repeat the same block-spin transformation step by step.

3.2. Antiferromagnetic Order Parameter

For the AF order parameter, one should take account of the two-sublattice structure. Three components of the order parameter are defined as follows:

\[
q_\sigma = \left( \sum_{i \in A} \delta_{S_i, \sigma} - \sum_{j \in B} \delta_{S_j, \sigma} \right) / N, \tag{2}
\]

where \(\sigma\) denotes one of the three states 0, 1 and 2, and \(A\) and \(B\) stand for two sublattices. Three states 0, 1, and 2 for the sublattices \(A\) and \(B\) can be expressed by two-dimensional vectors as shown in the inset of Fig. 2. It should be noted here that each pair of the neighboring vectors make an angle of \(\pi/3\); as a result, the order-parameter space in this case has a six-fold symmetry in contrast to that of the F Potts model. This symmetry, \(Z(6)\), is the same as that of the six-clock model. Based on this observation, we make block spins so as to preserve this six-fold symmetry; more specifically, as the block spin we choose one of the possible states of the six-clock spin which directs closest to the vector sum of the Potts spins in a block. Possible vectors obtained by the vector sum of eight Potts spins are illustrated in Fig. 2. At the border, a block spin should be chosen in equal probability by the random number. At the center, on the other hand, a block spin is chosen with the probability of 1/6.

We have chosen the primary direction of the six-clock spin as shown in Fig. 2. The reason is as follows: We expect that the ordered state of the AF three-state Potts model has a broken-sublattice-symmetry order.\(^{21,22}\) Namely, one sublattice is occupied by one of the three states, while the other sublattice is randomly occupied by the remaining two states. The present choice of the spin direction takes this type of order into account.

The block-spin transformation described above for the AF order cannot be expressed as a simple majority rule in contrast to the F case. Therefore, we must perform the vector summation directly. The multi-spin coding technique is applicable even in this case, since all the operations can be executed only with integer variables space. When the oblique coordinates are used for expressing the order-parameter space. The six states, 0, 1, 2, 3,
Fig. 2. Possible vectors obtained by the vector sum of eight AF Potts spins.

4, 5 in Fig. 2, are expressed by (000), (001), (101), (100), (111), (011) respectively in our binary-number representation. We use the basis vectors $e_x$ and $e_y$ shown in Fig. 2. Then, 0, 1 and 2 states on the sublattice $A$ are expressed by $r_A, e_x + r_A$ and $e_y + r_A$, respectively, where $r_A = (e_x + e_y)/3$. On the other hand, 0, 1 and 2 states on the sublattice $B$ are expressed by $e_x + e_y + r_B, e_y + r_B$ and $e_x + r_B$, respectively, where $r_B = 2(e_x + e_y)/3$.

The FORTRAN code of the block-spin transformation from the AF Potts spin to the six-clock spin is given as follows:

```fortran
cc block spin transformation
cc antiferro 3-state Potts to 6-clock
cc x>0 (icx = 0) or x=0 (icx = 1) or x<0 (icx = 2)
c icsumx =<< 4
c
   iwk = ior(icsumx0,icsumx1)
   icx0 = iand(icsumx2,not(iwk))
   icx1 = not(ior(icsumx2,icsumx3))

cc y>0 (icy = 2) or y=0 (icy = 1) or y<0 (icy = 0)
c icsumy =<< 4
c
   iwk = ior(icsumy0,icsumy1)
   icy0 = iand(icsumy2,not(iwk))
   icy1 = iand(ior(icsumy2,icsumy3),not(icy0))

cc icsumy + icsumx (0-16)
```
The sum of the $x$- and $y$-components of eight Potts spins are given by $isumx$ and $isumy$. 

```c
icr0 = iand(isumy0,isumx0)
isumC0 = ieor(isumy0,isumx0)
iwk = ieor(isumy1,isumx1)
icr1 = ieor(iand(isumy1,isumx1),iand(icr0,iwk))
isumC1 = ieor(icr0,iwk)
iwk = ieor(isumy2,isumx2)
icr2 = ieor(iand(isumy2,isumx2),iand(icr1,iwk))
isumC2 = ieor(icr1,iwk)
iwk = ieor(isumy3,isumx3)
isumC3 = ieor(icr2,iwk)
isumC4 = ieor(iand(isumy3,isumx3),iand(icr2,iwk))
```

c $y+x>0$ (icm = 2) or $y+x=0$ (icm = 1) or $y+x<0$ (icm = 0)
c $isumy + isumx \geq 8$
c
```
iwk = ior(isumC0,ior(isumC1,isumC2))
icm0 = iand(isumC3,not(iwk))
icm1 = iand(ior(isumC3,isumC4),not(icm0))
```

c if border
c
```
iran = ira(la)
```

c $icb2 = ior(icm1,iand(icm0,iran))$
iwk1 = ior(icx1,iand(icx0,iran))
iwk2 = ior(icy1,iand(icy0,iran))
icb1 = iand(iwk1,iwk2)
icb0 = not(ior(iwk1,iwk2))

c if center
c
```
icent = iand(icx0,iand(icy0,icm0))
nocent = not(icent)
ic2 = irb(la)
ic1 = not(ior(irt1(la),iran))
irt1(la) = ic1
ic0 = iand(not(irt0(la)),iran)
irt0(la) = ic0
```

c $isblk2(la) = ior(iand(nocent,icb2),iand(icent,ic2))$
isblk1(la) = ior(iand(nocent,icb1),iand(icent,ic1))
isblk0(la) = ior(iand(nocent,icb0),iand(icent,ic0))$
The conditions needed for the determination of the block spin are represented in terms of the conditions on $isum_x$, $isum_y$ and $isum_x+isum_y$, which are illustrated in Fig. 3. According to these conditions, the three words to denote the six-clock spin, $(isblk2, isblk1, isblk0)$, are determined by logical commands. The choice of the state at the border is simply made by the random number $ira$ with the probability of 1/2. At the center, on the other hand, we use two random numbers, $ira$ and $irb$: First, $isblk2$ is determined by the random number $irb$; next, the same procedure is employed for the determination of the three states represented by $isblk1$ and $isblk0$ as we used in choosing a trial state in the Monte Carlo update. The information of the selected state, $(irt1, irt0)$, is kept up to the next time. With this procedure, we can pick up one state from six with the equal probabilities.

Once the block spin having a six-fold symmetry is obtained, the next step will be the transformation from the six-clock spin to the block spin of the same symmetry. The illustration of this transformation is given in Fig. 4. Ties at the border and the center are treated similarly as before. We can apply the multi-spin coding technique also to the block-spin transformation from the six-clock spin to the six-clock block spin as before. Although we do not show the FORTRAN code for this transformation, it is worthwhile to make one comment: This time it is convenient to use basis vectors $e_{x'}$ and $e_{y'}$ shown in Fig. 4. Then, the six states 0, 1, 2, 3, 4 and 5 are represented respectively by $2e_{x'} + e_{y'} + r$, $2e_{x'} + 2e_{y'} + r$, $e_{x'} + 2e_{y'} + r$, $e_{y'} + r$, $r$ and $e_{x'} + r$ with $r = e_{x'} + e_{y'}$. The conditions in terms of $isumx-2*isumy$, $2*isumx-isumy$ and $isumx+isumy$ will be used for the determination of the block six-clock state.

4. Summary and Discussions

We have presented the multi-spin coding for the Monte Carlo simulation of the three-state Potts model. The multi-spin coding technique has also been applied to the block-spin transformations of the Potts model both with the F and AF order parameters. The emphasis should be put on the fact that we have totally excluded if-statement in our code; as a result, the code can perform ultrafast computations.

As we have mentioned in the Introduction, some earlier applications of the multi-spin coding for the Ising model as well as a recent one showed how to store several spins belonging to the same lattice in a word. This type of coding is effective for saving the
memory of computers. But not so dramatic acceleration in the simulation speed is expected. On the other hand, the method we have presented is based on yet another type of the multi-spin coding, which was originally proposed by Bhanot et al. for the Ising model and modified by Michael. In these methods and the present one as well, the multi-spin coding technique is used in order that a number of independent systems are simulated simultaneously. These simultaneous simulation methods do not help reducing the memory consumption; but we can expect a great reduction in the computation time. Since the memory restriction is getting more and more relaxed these days, the simultaneous simulation technique is advantageous over the earlier multi-spin coding methods. A simultaneous simulation method using 3 bits/spin coding has also been used for the Ising model a decade ago.

A short comment will be made here on the performance of the present code. We have achieved the speed of 0.81 G Potts-spin flips per second without any measurement in the case of 32-bits multi-spin coding of the 3D Potts model for periodic boundary conditions on the HITAC S-3800/480 system at the Computer Center of University of Tokyo. This is comparable to the speed of 2.10 G spin flips per second for the 3D Ising model on the same machine: For the 3D Potts model the number of the logical commands for a spin update is 110, which is about four times of that for the 3D Ising model. With the measurement of the energy and the magnetization, the performance for the 3D Potts model is changed to 0.49 G spin flips per second: When one makes block-spin transformations three times with the measurement of block-spin magnetizations, the speed becomes 0.44 G spin flips per second. We should note that the present code can be extended to the case of four-state Potts model, five-state Potts model, and so on, although the coding will be more cumbersome.

Using this fast code, we have investigated several interesting topics of the Potts model. The order-parameter distribution functions of the three-state Potts model has been studied in 2D and 3D where attention has been paid to the vector character of the order...
parameter. We have also treated the 3D AF Potts model for a careful study of the critical phenomena, using the MCRG method combined with finite-size scaling analysis; we have confirmed that the 3D AF three-state Potts model is in the $XY$ universality class within statistical errors.\footnote{1,6,25,26}

Another problem is the random three-state Potts model in 3D. We have studied the $\pm J$ model with general asymmetric probability weights. The overall phase diagram of the random Potts model as a function of the concentration of coupling and the temperature has been obtained. In the AF-rich region, we have paid attention to the universality of critical phenomena. We have also shown the rounding of the first-order transition due to the randomness in the F-rich region.\footnote{27,28}

The details of the physical results are given in each publication.\footnote{24,25,26,27,28}

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Appendix A

c Multi-Spin coding of the 3-dimensional 3-state Potts model
   with ferromagnetic (F), antiferromagnetic (AF)
   and random couplings

c subroutine sbltce(isp0,isp1,jx,jyr,jyl,jzr,jzl,ira,irb,iengd)
parameter(nx=64,nx2=nx/2,nxy2=nx2*nx,nla2=nxy2*nx)
parameter(nword=2**24)
common/jxtab/jxtb0(0:nword-1),jxtb1(0:nword-1)
   ,jxtb2(0:nword-1)
dimension isp0(0:nla2-1,0:1),isp1(0:nla2-1,0:1)
dimension jx(0:nla2-1),jyr(0:nla2-1),jyl(0:nla2-1)
   ,jzr(0:nla2-1),jzl(0:nla2-1)
dimension ira(0:nla2-1),irb(0:nla2-1)
dimension iengd(0:nla2-1,0:3)

   do 10 la=0,nla2-1

   c old spin -> isold

   isold0 = isp0(la,0)
isold1 = isp0(la,1)

   c set trial new spin -> isnew

   iscoina = ira(la)
isnew0 = iand(not(isold0),iscoina)
isnew1 = not(ior(isold1,iscoina))

   c energy difference for spin 1 -> ide1

   ide1 = iengd(la,0)
   ide2 = iengd(la,1)
   ide3 = iengd(la,2)
   ide4 = iengd(la,3)

10 continue
c neq : flag to tell whether n.n. spins are
the same (0) or not (1)
c ide : e(old) - e(new) + 1
neqold < neqnew then ide = 0 (2) for F (AF)
neqold = neqnew then ide = 1
neqold > neqnew then ide = 2 (0) for F (AF)
Note that (neqold = 0) and (neqnew = 0) are not realized
at the same time.

    is0 = isp1(la,0)
is1 = isp1(la,1)
neqold = ior(ieor(isold0,is0),ieor(isold1,is1))
neqnew = ior(ieor(isnew0,is0),ieor(isnew1,is1))
ide10 = iand(neqold,neqnew)
* for F :
    ide11 = not(neqnew)
* for AF :
    * ide11 = not(neqold)
* for random :
    * ide11 = ior(iand(jbond,not(neqnew)),not(ior(jbond,neqold)))

energy difference for spin 2 -> ide2

    is0 = isp1(jx(la),0)
is1 = isp1(jx(la),1)
neqold = ior(ieor(isold0,is0),ieor(isold1,is1))
neqnew = ior(ieor(isnew0,is0),ieor(isnew1,is1))
ide20 = iand(neqold,neqnew)
ide21 = not(neqnew)
* ide21 = not(neqold)
* ide21 = ior(iand(jbond,not(neqnew)),not(ior(jbond,neqold)))

energy difference for spin 3 -> ide3

    is0 = isp1(jyr(la),0)
is1 = isp1(jyr(la),1)
neqold = ior(ieor(isold0,is0),ieor(isold1,is1))
neqnew = ior(ieor(isnew0,is0),ieor(isnew1,is1))
ide30 = iand(neqold,neqnew)
ide31 = not(neqnew)
* ide31 = not(neqold)
* ide31 = ior(iand(jbond,not(neqnew)),not(ior(jbond,neqold)))

energy difference for spin 4 -> ide4
is0 = isp1(jyl(la),0)
is1 = isp1(jyl(la),1)
neqold = ior(ieor(isold0,is0),ieor(isold1,is1))
neqnew = ior(ieor(isnew0,is0),ieor(isnew1,is1))
ide40 = iand(neqold,neqnew)
ide41 = not(neqnew)
* ide41 = not(neqold)
* ide41 = ior(iand(jbond,not(neqnew)),not(ior(jbond,neqold)))

c energy difference for spin 5 -> ide5

is0 = isp1(jzr(la),0)
is1 = isp1(jzr(la),1)
neqold = ior(ieor(isold0,is0),ieor(isold1,is1))
neqnew = ior(ieor(isnew0,is0),ieor(isnew1,is1))
ide50 = iand(neqold,neqnew)
ide51 = not(neqnew)
* ide51 = not(neqold)
* ide51 = ior(iand(jbond,not(neqnew)),not(ior(jbond,neqold)))

c energy difference for spin 6 -> ide6

is0 = isp1(jzl(la),0)
is1 = isp1(jzl(la),1)
neqold = ior(ieor(isold0,is0),ieor(isold1,is1))
neqnew = ior(ieor(isnew0,is0),ieor(isnew1,is1))
ide60 = iand(neqold,neqnew)
ide61 = not(neqnew)
* ide61 = not(neqold)
* ide61 = ior(iand(jbond,not(neqnew)),not(ior(jbond,neqold)))

c sum of energy differences for 2 spins

isuma0 = ieor(ide10,ide20)
isuma1 = ior(ieor(ide11,ide21),iand(ide10,ide20))
isuma2 = iand(ide11,ide21)
isumb0 = ieor(ide30,ide40)
isumb1 = ior(ieor(ide31,ide41),iand(ide30,ide40))
isumb2 = iand(ide31,ide41)
isumc0 = ieor(ide50,ide60)
isumc1 = ior(ieor(ide51,ide61),iand(ide50,ide60))
isumc2 = iand(ide51,ide61)

c isuma = isuma + 2
isuma2 = ior(isuma1,isuma2)
isuma1 = not(isuma1)

c isumw = isuma + isumb

isumw0 = ieor(isuma0,isumb0)
icr = iand(isuma0,isumb0)
iwk= ieor(isuma1,isumb1)
isumw1 = ieor(iwk,icr)
icr = ior(iand(isuma1,isumb1),iand(iwk,icr))
iwk= ieor(isuma2,isumb2)
isumw2 = ieor(iwk,icr)
isumw3 = ior(iand(isuma2,isumb2),iand(iwk,icr))

c icr = iand(isumw0,isumc0)
icr = ior(iand(isumw1,isumc1),iand(iwk,icr))
icr = ior(iand(isumw2,isumc2),iand(iwk,icr))
isum3 = ior(isumw3,icr)

c isum = isumw + isumc

c isum : total trial energy difference (old-new) +8

c (2 <= isum <= 14)

isum0 = ieor(isumw0,isumc0)
icr = iand(isumw0,isumc0)
iwk= ieor(isumw1,isumc1)
isum1 = ieor(iwk,icr)
icr = ior(iand(isumw1,isumc1),iand(iwk,icr))
iwk= ieor(isumw2,isumc2)
isum2 = ieor(iwk,icr)
icr = ior(iand(isumw2,isumc2),iand(iwk,icr))
isum3 = ior(isumw3,icr)

jxtb : X-table for Boltzmann factor

(0 <= jxtb <= 6)
c iflip : flag for spin flip

c isum + jxtb >= 8 then flip

ir = irb(la)
jt0 = jxtb0(ir)
jt1 = jxtb1(ir)
jt2 = jxtb2(ir)
icr = iand(ieor(isum1,jt1),iand(isum0,jt0))
icr = ior(iand(isum1,jt1),icr)
icr = iand(ieor(isum2,jt2),icr)
icr = ior(iand(isum2,jt2),icr)
iflip = ior(isum3,icr)

c new spin -> isp0(la)
isp0(la,0) = ior(iand(iflip,isnew0),iand(not(iflip),isold0))
isp0(la,1) = ior(iand(iflip,isnew1),iand(not(iflip),isold1))

c  energy difference (old-new) + 8  (2 <= iengd <= 14)
    iengd(la,0) = iand(iflip,isum0)
    iengd(la,1) = iand(iflip,isum1)
    iengd(la,2) = iand(iflip,isum2)
    iengd(la,3) = ior(not(iflip),isum3)

10 continue

end