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1  module general                                !General Module to be used everywhere
2      integer, allocatable :: x(:)             !list of n particles
3      integer :: n                             !no. of particles
4  end module
5
6  program Ising_Model
7      use general
8      implicit none
9      integer :: nmc, i, k, a
10     real :: J, B, kb, T, r, uold, unew, du, w, utot
11     J = 1.0;      B = 0.0;      kb = 1.0;      T = 0.7
12     nmc = 500000;      n = 1000
13     allocate(x(n))
14     do i = 1, n
15         x(i) = 1
16     enddo
17     open(1, file = "result.dat");      open(2, file = "States.dat")
18     write(2, *) "Initial State"
19     write(2, *) x
20     call total_energy(J, B, utot)
21 !Energy,      Energy per Spin,      Magnetization,      Magnetization per Spin
22     write(1, *) utot, utot/n, real(sum(x)), real(sum(x))/(n*1.0)
23
24     do i = 1, nmc
25         do k = 1, n
26
27             call random_number(r)
28             a = int(r*n) + 1
29             if (a > n) then
30                 a = n
31             endif
32
33             call energy(J, B, a, uold)
34             x(a) = -x(a)
35             call energy(J, B, a, unew)
36
37             if(unew > uold) then
38                 du = unew - uold
39                 w = exp(-du/(kb*T))
40                 call random_number(r)
41                 if(r >= w) then
42                     x(a) = -x(a)
43                 endif
44             endif
45         enddo
46
47         call total_energy(J, B, utot)
48         write(1, *) utot, utot/n, real(sum(x)), real(sum(x))/(n*1.0)
49     enddo
50
51     write(2, *) "Final State"
52     write(2, *) x
53
54 end program
55
56 ! E = -J * Sum(Si*Sj) - B * Sum(Si)
57
58 subroutine energy(j, b, i, u)      !Calculate total energy of given State
59     use general
60     implicit none
61     integer :: i
62     real :: d, u, j, b, e
63     u = 0.0
64     if(i == 1) then
65         e = -j*x(i)*(x(n) + x(i-1)) - b*x(i); u = u + e
66     elseif(i == n) then

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67         e = -j*x(i)*(x(1) + x(i-1)) - b*x(i); u = u + e
68     else
69         e = -j*x(i)*(x(i-1) + x(i+1)) - b*x(i); u = u + e
70     endif
71     return
72 end subroutine
73
74 subroutine total_energy(j,b,u)
75     use general
76     implicit none
77     integer::i
78     real::d,u,j,b,e
79     u = 0.0
80     do i = 1,n
81         if(i == n) then
82             e = -j*(x(n)*x(1)); u = u + e
83         else
84             e = -j*(x(i)*x(i+1)); u = u + e
85         endif
86         u = u - b*sum(x)
87     enddo
88     return
89 end subroutine

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