3D Ising model

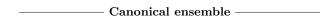
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The Ising Model

Let consider a Lattice of dimension $n \times m \times l$ where we each point on the can have spin up, $\sigma = 1$, or down, $\sigma = -1$, representing for example the spin orientation of a ferromagnetic material. We then attribute a binding-energy, J, to the bond between each of the adjacent neighbor of a lattice point and a mean energy of h, called the chemical potential, representing the attribution of a external magnetic field.

In statistical physics we are able to calculate certain properties of such materials but for this we will need the partition function.



Lets consider a system where the number of particles, N, and the systems volume, V, is held constant. Lets assume that the system is isolated and in thermal equilibrium with a heat bath at a certain temperature, T. For such a system the partition function is given as the follow sum

$$Z_C(V, T, N) = \sum_{s} \exp(-\beta H(N, s)),$$

where s is the index for the microstates of the system, β is the thermodynamic beta defined as $\frac{1}{k_BT}$, where k_B is the Boltzmann constant, and H(N,s) is the Hamiltonian of the system with N particles in the respective microstate. Such a system where N, V, and T are held constant is called a canonical ensemble and its partition function the canonical partition function, denoted $Z_C(V,T,N)$.

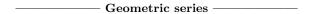


Lets consider the same system as above but with the difference that the system now can exchange particle with the reservoir.

For such a system the partition function is just given as the sum of all possible canonical partition function

$$Z_G(V, T, h) = \sum_{N,s} \exp(-\beta H(N, s)) = \sum_N Z_C(V, T, N)$$

Such a system where h, V, and T are held constant is called a grand canonical ensemble and its partition function the grand canonical partition function, denoted $Z_G(V, T, h)$.



In mathematics, a geometric series can be proven fulfill the following relation

$$\sum_{k=0}^{\infty} r^k = \frac{1}{1-r}, \quad \text{if} \quad |r| < 1.$$

rewriting a bit we get

$$\sum_{k=1}^{\infty} r^k = \sum_{k=0}^{\infty} r^k - 1$$

$$= \frac{1}{1-r} - 1, \text{ if } |r| < 1,$$

$$= \frac{r}{1-r}.$$

Also note worthy is that if we differentiate both sides of the geometric series we get

$$\sum_{k=1}^{\infty} kr^{k-1} = \frac{1}{(1-r)^2}, \quad \text{if} \quad |r| < 1,$$

giving in tern

$$\sum_{k=1}^{\infty} kr^k = \frac{r}{(1-r)^2}, \quad \text{if} \quad |r| < 1.$$

Combining these we get

$$\frac{\sum_{k=1}^{\infty} kr^k}{\sum_{k=1}^{\infty} r^k} = \frac{\frac{r}{(1-r)^2}}{\frac{r}{1-r}} = \frac{1}{1-r}, \quad \text{if} \quad |r| < 1.$$

Eigen Decomposition —

Let A be a square $(n \times n)$ matrix with n linearly independent eigenvectors, q_i (i = 1, ..., n). Then A can be factorized as

$$\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{-1}$$

where Q is the square $(n \times n)$ matrix whose i'th column is the eigenvector q_i of A and Λ is the diagonal matrix whose diagonal elements are the corresponding eigenvalues, i.e., $\Lambda_{ii} = \lambda_i$. Note that only diagonalizable matrices can be factorized in this way. - source: wiki

Then

$$\mathbf{A}^{N} = (\mathbf{Q}\Lambda\mathbf{Q}^{-1})^{N}$$

$$= \mathbf{Q}\Lambda\mathbf{Q}^{-1}\mathbf{Q}\Lambda\mathbf{Q}^{-1}\cdots\mathbf{Q}\Lambda\mathbf{Q}^{-1}$$

$$= \mathbf{Q}\Lambda\Lambda\cdots\Lambda\mathbf{Q}^{-1}$$

$$= \mathbf{Q}\Lambda^{N}\mathbf{Q}^{-1},$$

where we used that $\mathbf{Q}^{-1}\mathbf{Q} = 1$. Note also that

$$\mathbf{\Lambda}^{N} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}^{N} = \begin{pmatrix} \lambda_1^{N} & 0 & \cdots & 0 \\ 0 & \lambda_2^{N} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^{N} \end{pmatrix},$$

thus

$$\begin{split} \operatorname{Tr} \big[\mathbf{A}^N \big] &= \operatorname{Tr} \big[\mathbf{Q} \mathbf{\Lambda}^N \mathbf{Q}^{-1} \big] \\ &= \operatorname{Tr} \big[\mathbf{Q} \big] \operatorname{Tr} \big[\mathbf{\Lambda}^N \big] \operatorname{Tr} \big[\mathbf{Q}^{-1} \big] \\ &= \operatorname{Tr} \big[\mathbf{Q} \big] \sum_{i=1}^n \lambda_i^N \operatorname{Tr} \big[\mathbf{Q}^{-1} \big] \\ &= \sum_{i=1}^n \lambda_i^N \operatorname{Tr} \big[\mathbf{Q} \mathbf{Q}^{-1} \big] \\ &= \sum_{i=1}^n \lambda_i^N. \end{split}$$

Since $\mathbf{A} \in \mathbf{M}_{n \times n}$, we will have n eigenvalues λ_i and one of these $\lambda_l \equiv \lambda_{max} > \lambda_i$, $\forall i \in [1:n] \setminus \{l\}$. So we can approximate the magnetization to

$$\lim_{N \to \infty} \operatorname{Tr} \left[\mathbf{A}^N \right] = \sum_{i=1}^n \lambda_i^N = \lambda_{max}^N.$$

————— Physical quantities ————

Once the partition function for a system is obtain it is possible to calculate a plethora of observable quantities. For example with the grand canonical partition function we can calculate the average magnetization of the lattice as a function of temperature

$$m = \langle \sigma_0 \rangle = \frac{1}{\beta} \left(\frac{\partial \ln Z_G}{\partial h} \right)_{T,V} = \frac{1}{\beta} \frac{1}{Z_G} \frac{\partial Z_G}{\partial h}.$$
 (1)

Sometimes defined as

$$m = \langle \sigma_0 \rangle = -\frac{1}{N} \frac{\partial G}{\partial h}, \text{ where } G = -k_B T \ln Z_G.$$

Lets look at this derivative, assuming we can write $\frac{\partial}{\partial \mu} Z_G(V, T, C) = \beta N Z_C(V, T, N)$ which is often the case,

$$\frac{\partial Z_G}{\partial \mu} = \sum_N \frac{\partial}{\partial \mu} Z_C(V, T, N) = \sum_N \beta N Z_C(V, T, N).$$

This gives

$$m = \frac{1}{Z_G} \sum_{N} N Z_C(V, T, N). \tag{2}$$

Assuming further that we can write $Z_C(V, T, N) = Z_C(V, T, 1)^N$, which is the aim of this exercise to show can be done, then

$$m = \frac{1}{\sum_{N=1}^{\infty} (Z_C(V, T, 1))^N} \sum_{N=1}^{\infty} N(Z_C(V, T, N))^N = \frac{1}{1 - Z_C(V, T, 1)}, \quad \text{if} \quad |Z_C(V, T, 1)| < 1,$$

where we applied our result from the geometric series, shown above.

Assuming that $Z_C(V, T, N) = \text{Tr}[P^N]$, where P is a square diagonal matrix, we get the approximate magnetization

$$m \simeq \frac{1}{1 - \lambda_{max}}, \quad \text{if} \quad |\lambda_{max}| < 1,$$

where we applied our result from eigendecomposition of a matrices, shown above.

———— One Dimensional model ————

We assume a nearest neighbor model of a chain of N particles with free ends subject to a non-zero external field. The resulting Hamiltonian for a particular microstate is

$$H(N,s) = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} - h \sum_{i=1}^{N-1} \sigma_i = -\sum_{i=1}^{N-1} \left(J \sigma_i \sigma_{i+1} + \frac{h}{2} (\sigma_i + \sigma_{i+1}) \right)$$

The resulting canonical partition function is

$$\begin{split} Z_C(V,T,N) &= \sum_s \exp(-\beta H(N,s)) \\ &= \sum_{j=1}^N \sum_{\sigma_j = \{-1,1\}} \prod_{i=1}^N e^{\left(J\sigma_i \sigma_{i+1} + \frac{h}{2}(\sigma_i + \sigma_{i+1})\right)} = \sum_{j=1}^N \sum_{\sigma_j = \{-1,1\}} \prod_{i=1}^N P_{\sigma_i \sigma_{i+1}} = \text{Tr} P^N \\ &= \lambda_1^N + \lambda_2^N, \quad \text{hvor} \quad P = \left(\begin{array}{cc} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J+h)} \end{array} \right). \end{split}$$

From linear algebra we know that the eigen values to $|P - \lambda I|$ are $\lambda = e^{\beta J} \cosh \beta h \pm \sqrt{e^{2\beta J} \sinh^2 \beta h + e^{-2\beta J}}$. Since $\lambda_1 > \lambda_2$ we will see in the thermodynamic limit that

$$G = -k_B T \ln Z_N = -k_B T \left(N \ln \lambda_1 + \ln \left[1 + \left(\frac{\lambda_2}{\lambda_1} \right)^N \right] \right) \to -Nk_B T \ln \lambda_1.$$

From this we can calculate the magnetization

$$m = \langle \sigma_0 \rangle = -\frac{1}{N} \frac{\partial G}{\partial h} = \frac{k_B T}{\lambda_1} \frac{\partial \lambda_1}{\partial h} = \frac{\sinh \beta h}{\sqrt{\sinh^2 \beta h + e^{-4\beta J}}}.$$

We see here that m=0 for h=0. But if $\sinh^2\beta h >> e^{-4\beta J}$ for $h\neq 0$ only a slight field, h, is needed for coherence to occur.

This non-zero field $(h \neq 0)$ would in the limit $G(T \to 0) = -NJ$ lead to a complete spin alignment and we can say that we have a phase transition for T = 0.

For $T \neq 0$ we would then have a analytical function for G which we didn't get in the "Men field theory" and Bragg-Williams approximation where we had discontinuity.

————— Two Dimensional model —————

We now consider the two dimensional Ising model constituting a $N \times N$ -lattice (se figur 16.10). For such a system we can write the Hamiltonian as

$$H(N,s) = -J \sum_{i=1}^{N} \sum_{j=1}^{N} [\sigma_{i,j}\sigma_{i+1,j} + \sigma_{i,j}\sigma_{i,j+1}] - h \sum_{i=1}^{N} \sum_{j=1}^{N} \sigma_{i,j}.$$

Assuming a periodic boundary condition, $\sigma_{i,j} = \sigma_{i+N,j} = \sigma_{i,j+N} = \sigma_{i+N,j+N}$, and introducing a column vector $\mu_j = (\sigma_{1,j}, \sigma_{2,j}, \dots, \sigma_{N,j})^T$ from which we denote the binding energy between two columns as E given as

$$E(\mu_j, \mu_k) = J \sum_{i=1}^{N} \sigma_{i,j} \sigma_{i,k} \quad \forall k \in \{j-1, j+1\},$$

since we assume we are only looking at nearest neighbors in any direction.

Further more we introduce the define the binding energy internally within a certain column to be ε given as

$$\varepsilon(\mu_j) = J \sum_{i=1}^{N} \sigma_{i,j} \sigma_{i+1,j} + h \sum_{i=1}^{N} \sigma_{i,j} \doteq -H_{1D}$$

Using these definitions we rewrite the Hamiltonian

$$H(N, \mu) = -\sum_{j=1}^{N} [E(\mu_j, \mu_{j+1}) + \varepsilon(\mu_j)],$$

and by introducing the matrix element $(P)_{\mu_j,\mu_k} = e^{\beta \left[E(\mu_j,\mu_k) + \frac{1}{2}(\varepsilon(\mu_j) + \varepsilon(\mu_k))\right]}$ we can write the partition function

$$Z_G(V, T, N) = \sum_{i=1}^{N} \sum_{\mu_i} e^{-\beta H(N, \mu)} = \sum_{i=1}^{N} \sum_{\mu_i} \prod_{j=1}^{N} (P)_{\mu_j, \mu_{j+1}}, \quad \text{hvor} \quad \sum_{\mu_j} = \sum_{l=1}^{N} \sum_{\sigma_{l,j} = -1}^{1},$$
$$= \text{Tr}[P^N] = \sum_{i}^{N} \lambda_i^N \approx \lambda_{max}^N, \quad n \to \infty,$$

where

$$P = \begin{pmatrix} (P)_{11\cdots 1,11\cdots 1} & (P)_{11\cdots 1,11\cdots -1} & \cdots & (P)_{11\cdots 1,-1-1\cdots -1} \\ (P)_{11\cdots -1,11\cdots 1} & (P)_{11\cdots -1,11\cdots -1} & \cdots & (P)_{11\cdots -1,-1-1\cdots -1} \\ \vdots & \vdots & \ddots & \vdots \\ (P)_{-1-1\cdots -1,11\cdots 1} & (P)_{-1-1\cdots -1,11\cdots -1} & \cdots & (P)_{-1-1\cdots -1,-1-1\cdots -1} \end{pmatrix}.$$

Since $P \in \mathbf{M}_{2^N \times 2^N}$ it will have 2^N eigenvalues λ_i and one of these $\lambda_l \equiv \lambda_{max} > \lambda_i$, $\forall i \in [1:n] \setminus \{l\}$.

From C. N. Yang 1952 get the exact solution, for $T < T_c$, where $k_B T_c \approx 2.269185 J$, since $2 \tanh^2 \frac{2J}{k_B T_c} = 1$. From Haung 1963:

$$g(0,T) = -k_B T \ln[2\cosh(2\beta J)] - \int_0^{\pi} d\phi \ln \frac{1}{2} \left(1 - \sqrt{1 - K^2 \sin^2 \phi}\right)$$

where $K = 2/[\cosh(2\beta J) \coth(2\beta J)]$ and

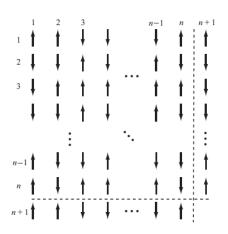
$$-\lim_{h\to 0}\frac{\partial g}{\partial h}=m=\left\{\begin{array}{cc}0&T>T_c\\\left\{1-\left[\sinh(2\beta J)\right]^{-4}\right\}^{\frac{1}{8}}&T< T_c\end{array}\right.$$

Further more we are able to calculate the heat capacity divergence near T_c . In figure 16.10 we see C_h for h = 0 hear $T = T_c$.

The divergence in C_h is logarithmic since we are working in a two dimensional model. In three dimensions we would expect a power series divergence.

In a similar way we can find the the other critical exponents for this two dimensional model

$$\beta = \frac{1}{8} \ (m), \quad \alpha = 0 \ (C), \quad \gamma = -\frac{7}{8} \ (\lambda).$$



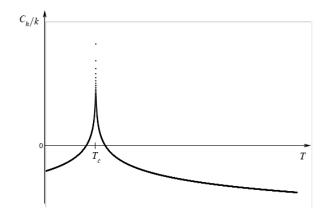


Fig. 16.9 Two-dimensional Ising system subject to periodic boundary conditions.

Fig. 16.10 Heat capacity of the two-dimensional Ising model (see eqn. (16.7.13)).

———— Three Dimensional model ————

We now consider the three dimensional Ising model constituting a $N \times N \times N$ -lattice. For such a system we can write the Hamiltonian as

$$H = -J \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} [\sigma_{i,j,k} \sigma_{i+1,j,k} + \sigma_{i,j,k} \sigma_{i,j+1,k} + \sigma_{i,j,k} \sigma_{i,j,k+1}] - h \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \sigma_{i,j,k}.$$

Assume periodic $\sigma_{i,j,k} = \sigma_{i+N,j,k} = \sigma_{i,j+N,k} = \sigma_{i,j,k+N} = \sigma_{i+N,j+N,k} = \dots$ Define a plane perpendicular to the z-axis in the lattice

$$\mu_{k} = \begin{pmatrix} \sigma_{1,1,k} & \sigma_{1,2,k} & \cdots & \sigma_{1,N,k} \\ \sigma_{2,1,k} & \sigma_{2,2,k} & \cdots & \sigma_{2,N,k} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{N,1,k} & \sigma_{2,N,k} & \cdots & \sigma_{N,N,k} \end{pmatrix}$$

Then the energy between two plates is

$$E(\mu_k, \mu_{k'}) = J \sum_{i=1}^{N} \sum_{j=1}^{N} \sigma_{i,j,k} \sigma_{i,j,k'} = 0 \quad \forall k' \in \{k-1, k+1\},$$

and the internal energy within a plate is

$$\varepsilon(\mu_k) = J \sum_{i=1}^{N} \sum_{j=1}^{N} [\sigma_{i,j,k} \sigma_{i+1,j,k} + \sigma_{i,j,k} \sigma_{i+1,j,k}] + h \sum_{i=1}^{N} \sigma_{i,j,k} \doteq -H_{2D}.$$

This means we can write the Hamiltonian as

$$H(N, h, T) = -\sum_{k=1}^{N} [E(\mu_k, \mu_{k+1}) + \varepsilon(\mu_k)].$$

Defining $(P)_{\mu_j,\mu_k} = e^{\beta \left[E(\mu_j,\mu_k) + \frac{1}{2}(\varepsilon(\mu_j) + \varepsilon(\mu_k))\right]}$ means intern we can simplifies the grand canonical partition function to

$$Z(H, h, T) = \sum_{i=1}^{N} \sum_{\mu_i} e^{-\beta H(N, h, T)} = \sum_{i=1}^{N} \sum_{\mu_i} \prod_{j=1}^{N} (P)_{\mu_j, \mu_{j+1}}, \quad \text{hvor} \quad \sum_{\mu_k} = \sum_{l=1}^{N} \sum_{m=1}^{N} \sum_{\sigma_{l, m, k} = -1}^{1};$$

$$= \text{Tr}[P^N] = \sum_{i}^{N} \lambda_i^N \approx \lambda_{max}^N, \quad N \to \infty,$$

since $P \in \mathbf{M}_{2^{N^2} \times 2^{N^2}}$, see appendix, we will have 2^{N^2} eigenvalues λ_i and one of these $\lambda_l \equiv \lambda_{max} > \lambda_i$, $\forall i \in [1:2^{N^2}] \setminus \{l\}$.

Now P as a matrix contains the exponential of the Hamiltonian, in units of k_BT , of all possible configuration of two adjacent plates in the lattice including the plates internal binding. For a $N^2 \times N$ lattice we can write P as

where I write 2 instead of -1 to save space. The specific case of an $2^2 \times N$ lattice is shown in the appendix.

With this solution we can calculate all the same critical exponentials in the same way as we did in the two dimensional case, either for the approximated or full solution. I haven't gotten so far yet. It would also be prudent to preform some Monte Carlo calculations to verify the results.

----- Transfer matrix -----

The transfer matrix has the form

$$P = \left[\begin{array}{c|c} A & B \\ \hline \tilde{I}B\tilde{I} & \tilde{I}A\tilde{I} \end{array} \right],$$

where $A,B,\tilde{I}\in\mathcal{M}_{2^{N^2-1}\times 2^{N^2-1}}$ and

$$\tilde{I} = \begin{pmatrix} 0 & 1 \\ & \ddots & \\ 1 & 0 \end{pmatrix}.$$

Such that e.g. $\tilde{I}A\tilde{I}$ results in an 180 degree rotation of the matrix A. This means that A and $\tilde{I}A\tilde{I}$ has the same eigenvalues, likewise for B and $\tilde{I}B\tilde{I}$. The largest eigenvalue of the transfer matrix can then be found by taking the sum of the eigenvalues of A and B.

For $N = \{3, 4, 5\}$ P will take up approximately $\{0.3MB, 4.3GB, 1126TB\}$ of memory alone. So N = 4 seems to be the computational limit of the early 21st century state of the art machines.

Appendix: $2 \times 2 \times N$ -lattice example

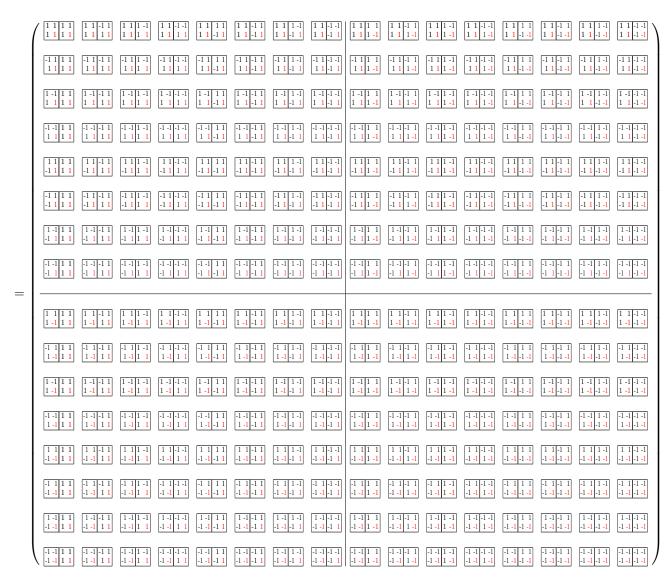
So P matrix represents all possible configuration of a plane or slice of the lattice perpendicular to the z-axis. So if we consider one slice of a $2 \times 2 \times N$ lattice and introduces the notation of a square represent one plane and the numbers inside representing a particular spin configuration in that plane. For example if all four particles in the first plane are aligned in the up direction.

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \doteq e^{\beta \varepsilon(\mu_1)}, \quad \text{where } \mu = \begin{pmatrix} \sigma_{111} = 1 & \sigma_{121} = 1 \\ \sigma_{211} = 1 & \sigma_{221} = 1 \end{pmatrix}$$
$$= J[4(11+11)] + h[4(1)]$$

Now we introduce the notation of two squares representing the coupling between planes

$$\frac{\left[\begin{array}{c} 1 & 1 \\ 1 & 1 \end{array}\right] \dot{=} \exp(\beta(E(\mu_1, \mu_2) + \varepsilon(\mu_1) + \varepsilon(\mu_2))), \quad \text{where} \quad \mu_1 = \begin{pmatrix} \sigma_{111} = 1 & \sigma_{121} = 1 \\ \sigma_{211} = 1 & \sigma_{221} = 1 \end{pmatrix} \quad \text{and} \quad \mu_2 = \begin{pmatrix} \sigma_{112} = -1 & \sigma_{122} = 1 \\ \sigma_{212} = 1 & \sigma_{222} = 1 \end{pmatrix} \\
= \exp\left(\beta\left(\left(-J[(1(-1)) + 3(11)]\right) + \left(J[4(11 + 11)] + h[4(1)]\right) + \left(J[4(1(-1) + 11)] + h[(-1) + 3(1)]\right)\right)\right)$$

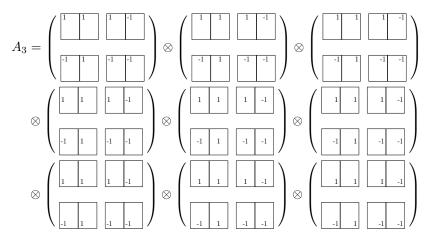
where we assigned two arbitrary configurations to the first and second plane. So if we consider the case of a $2 \times 2 \times N$ lattice we get



To convince yourself that this is indeed the solution to a three dimensional lattice try and do one random row/column multiplication from the product of $P^2 = P \times P$. Then you'll see products of the type

Note that all these are periodic and represent all possible combination with the $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ boundary condition in a 2^3 cube lattice. Indeed if one did the full calculation one would see that all the periodic solutions are on the diagonal of P^2 as it should, since we take the trace $\text{Tr}[P^N]$ for our periodic solution to the grand canonical partition function. This method can be expanded to any square size of the x/y-plane. For example in the case of a $3 \times 3 \times N$ -lattice we

have



and so on. A script could easily be devised to write this matrix to any square size the challenge is obtaining decomposition of a $2^{N^2} \times 2^{N^2}$ matrix. This challenge can be reduced by only obtaining the largest eigenvalue, but still.