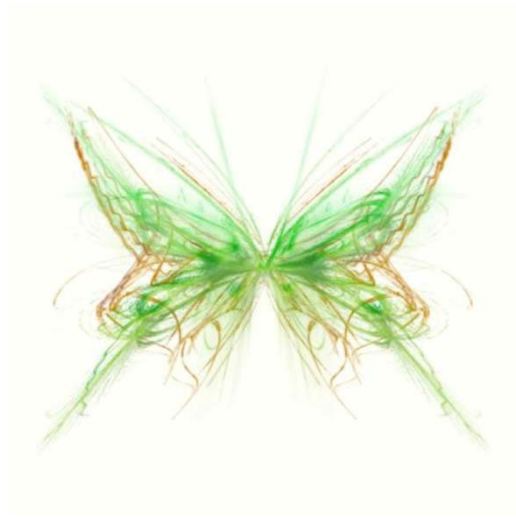
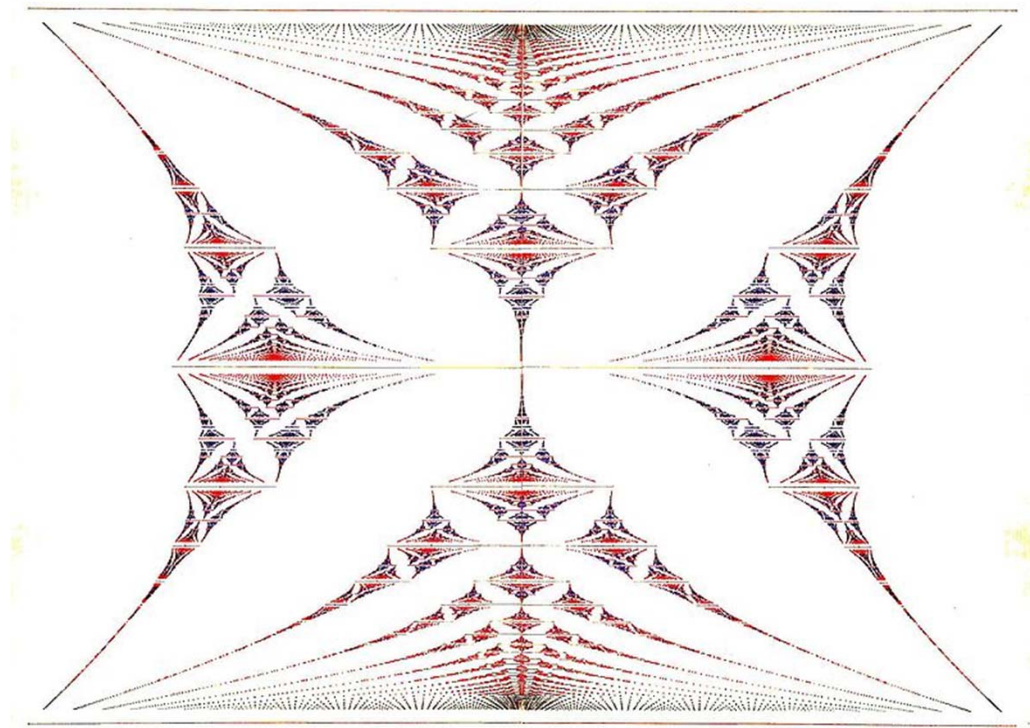




Hofstadter's

Butterfly



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Hofstadter's Butterfly

PHYSICAL REVIEW B

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Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields*

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(Received 9 February 1976)

An effective single-band Hamiltonian representing a crystal electron in a uniform magnetic field is constructed from the tight-binding form of a Bloch band by replacing $\hbar\vec{k}$ by the operator $\vec{p} - e\vec{A}/c$. The resultant Schrödinger equation becomes a finite-difference equation whose eigenvalues can be computed by a matrix method. The magnetic flux which passes through a lattice cell, divided by a flux quantum, yields a dimensionless parameter whose rationality or irrationality highly influences the nature of the computed spectrum. The graph of the spectrum over a wide range of "rational" fields is plotted. A recursive structure is discovered in the graph, which enables a number of theorems to be proven, bearing particularly on the question of continuity. The recursive structure is not unlike that predicted by Azbel¹, using a continued fraction for the dimensionless parameter. An iterative algorithm for deriving the clustering pattern of the magnetic subbands is given, which follows from the recursive structure. From this algorithm, the nature of the spectrum at an "irrational" field can be deduced; it is seen to be an uncountable but measure-zero set of points (a Cantor set). Despite these features, it is shown that the graph is continuous as the magnetic field varies. It is also shown how a spectrum with simplified properties can be derived from the rigorously derived

Hofstadter's Butterfly

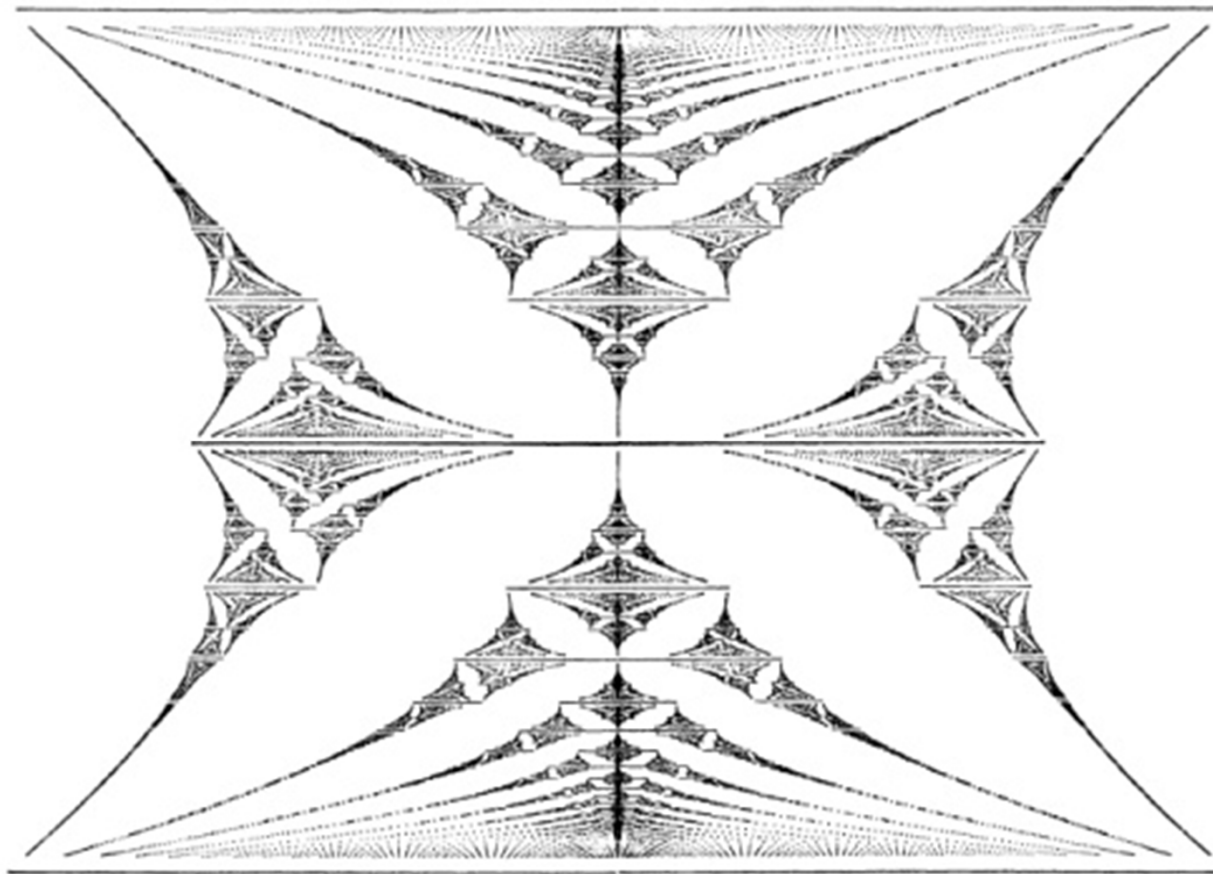
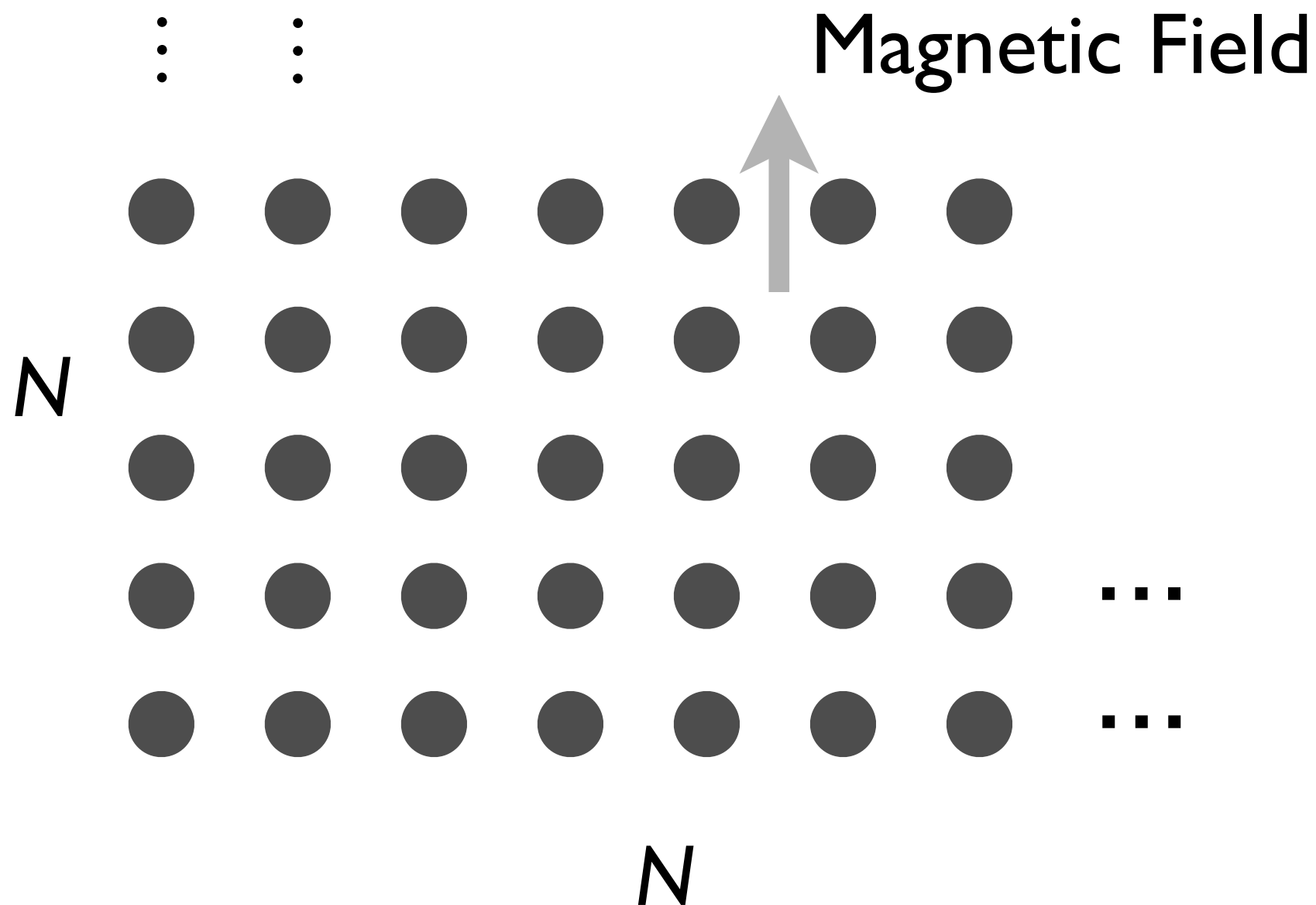


FIG. 1. Spectrum inside a unit cell. ϵ is the horizontal variable, ranging between $+4$ and -4 , and $\beta = \{\alpha\}$ is the vertical variable, ranging from 0 to 1 .

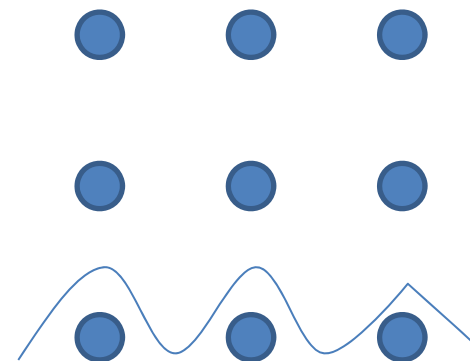
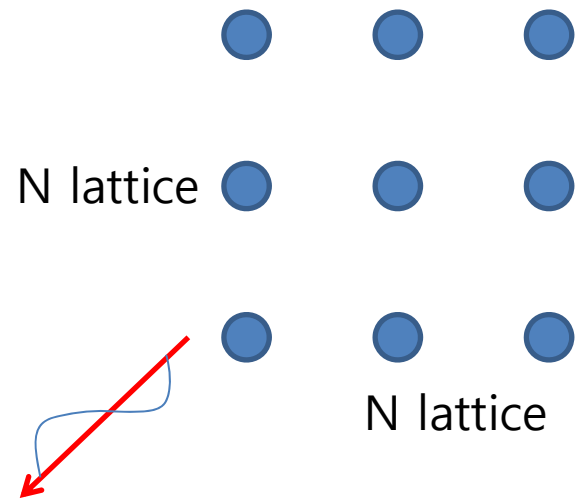
What did we do?

- Calculate the electron energy spectrum under periodic 2D potential + Strong magnetic field

- * Hamiltonian $\rightarrow N^2 \times N^2$ (sparse) matrix
- * Electron energy spectrum:
Eigenvalues of the Hamiltonian matrix

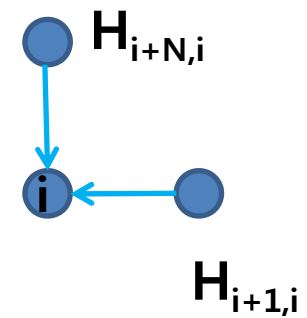
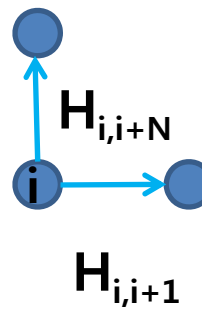
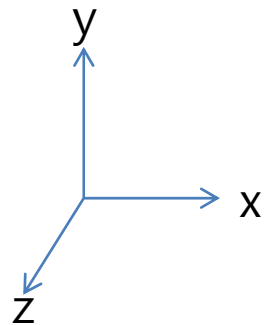


System

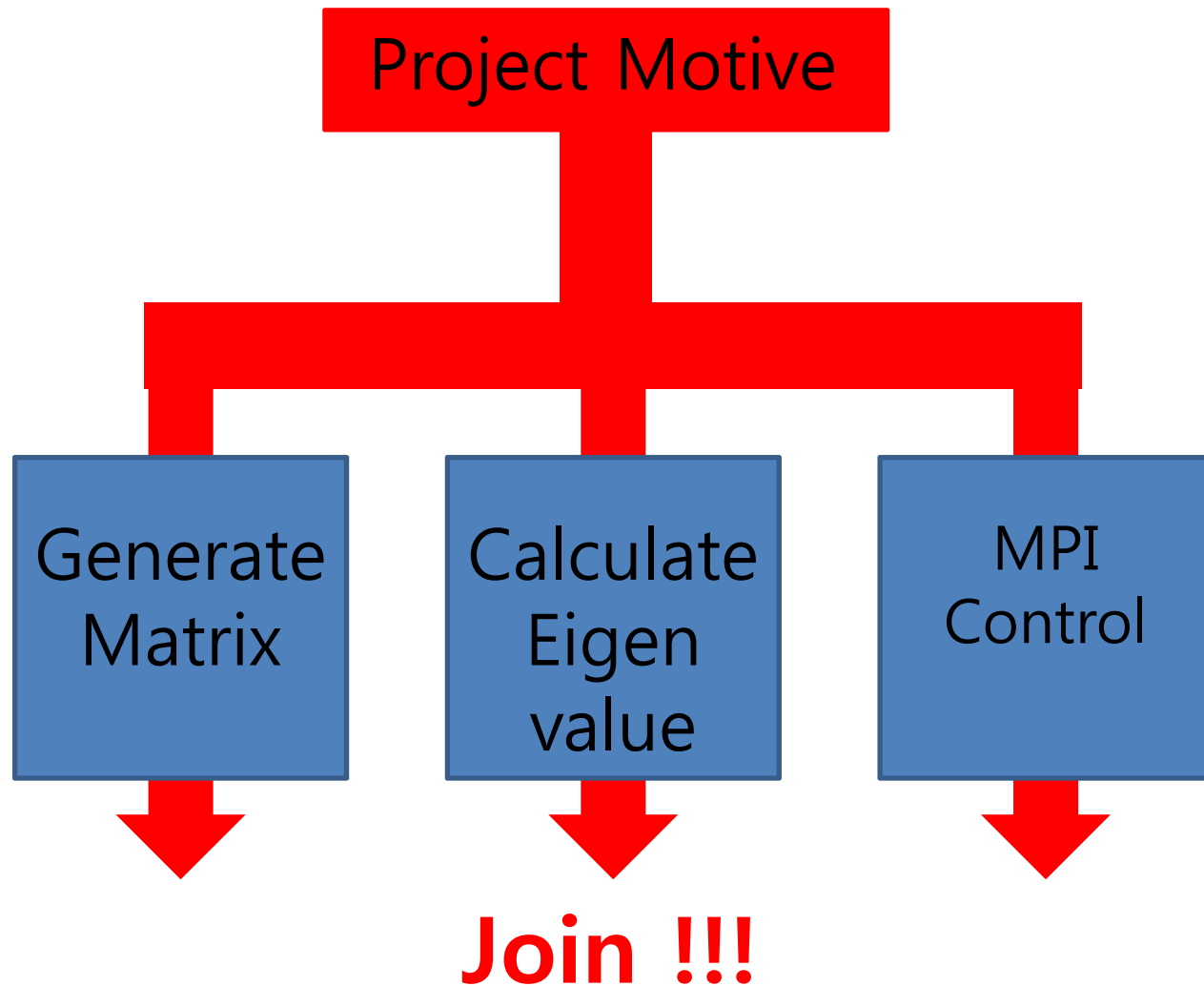


$i=1 \sim N^2$

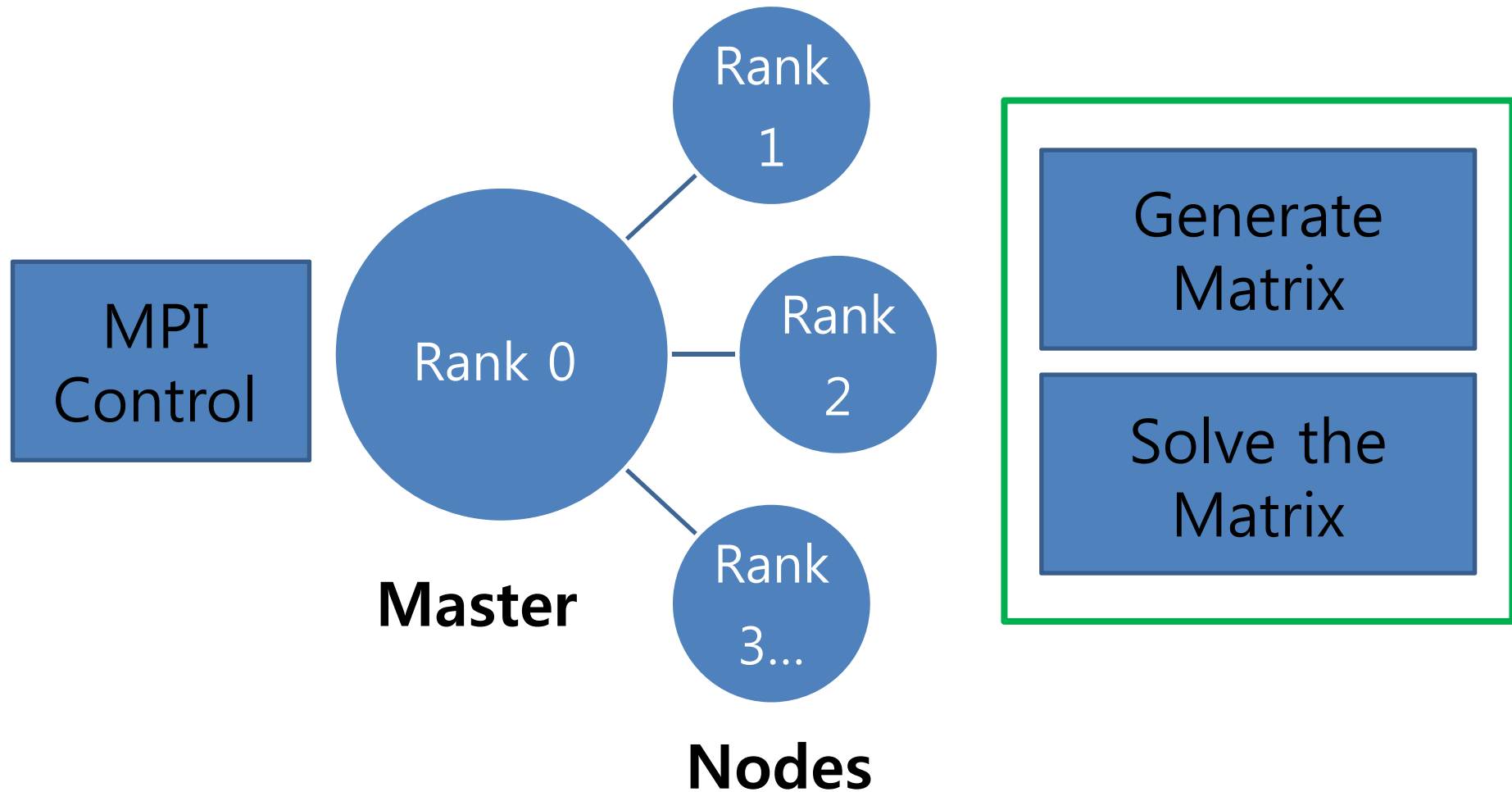
$$\langle j | H | i \rangle = H_{ij}$$

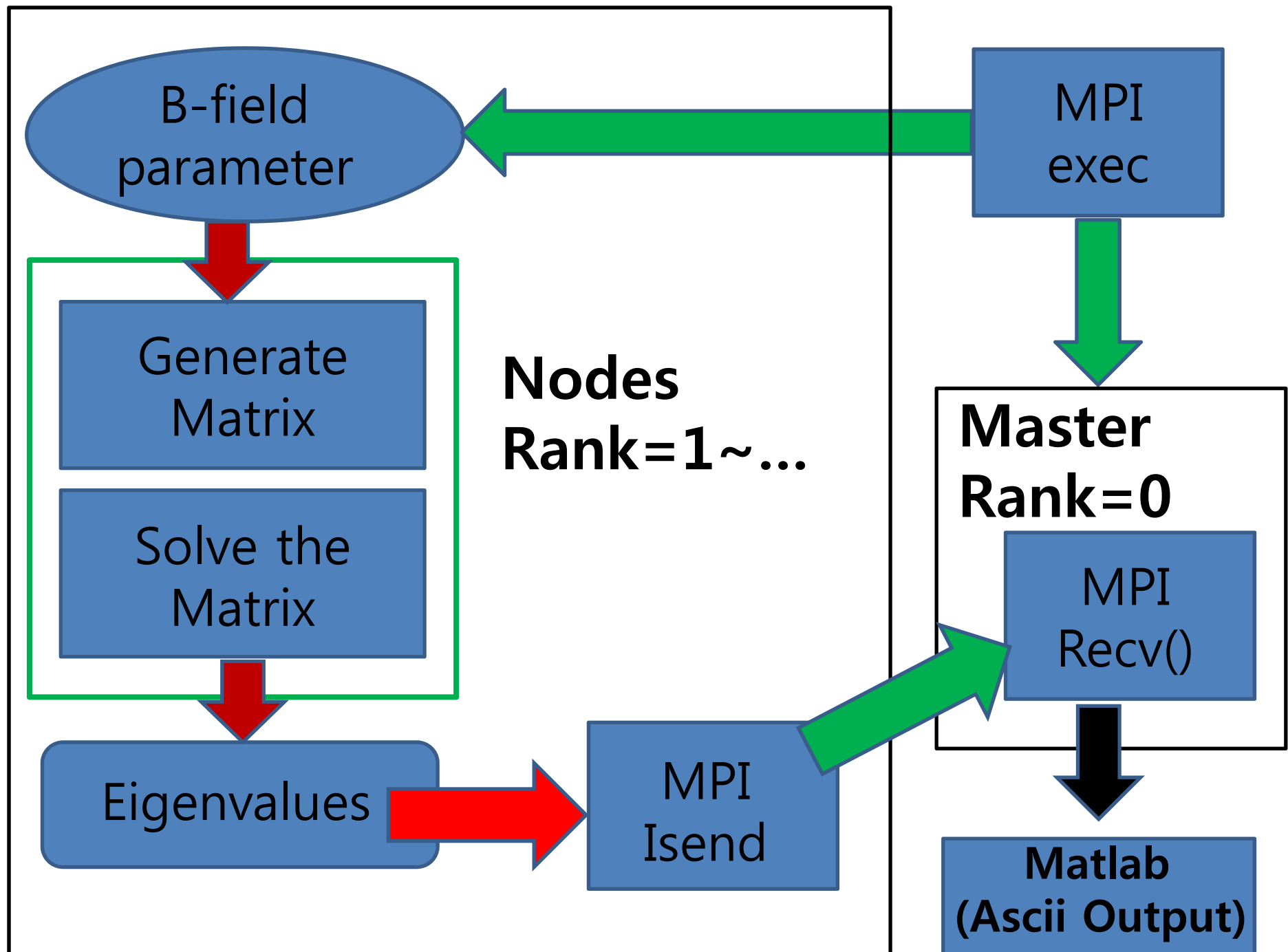


Member's Parallel Works



System Structure



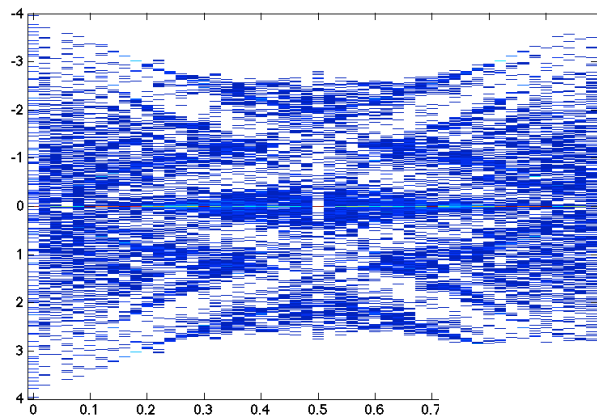


```

if (rank == 0) {
  for (i=N_cal; i<N_par; i++) {
    generate_matrix(i*interval);
    calculate_eigenvalue(ham, N_eig, eigen);
    ... (results <- eigen)
  }

  cnt = 0;
  while(cnt<N_cal){
    MPI_Recv(temp,N_eig, MPI_FLOAT, MPI_ANY_SOURCE, MPI_ANY_TAG,
             MPI_COMM_WORLD, &status);
    ... (results <- temp)
    cnt++;
  }
  print (results)
}
else {
  for (i=0; i<iter; i++) {
    generate_matrix(startparameter+interval*i);
    calculate_eigenvalue(ham, N_eig, eigen);
    MPI_Isend(eigen, N_eig, MPI_FLOAT, 0, rank, MPI_COMM_WORLD, &req1);
  }
}

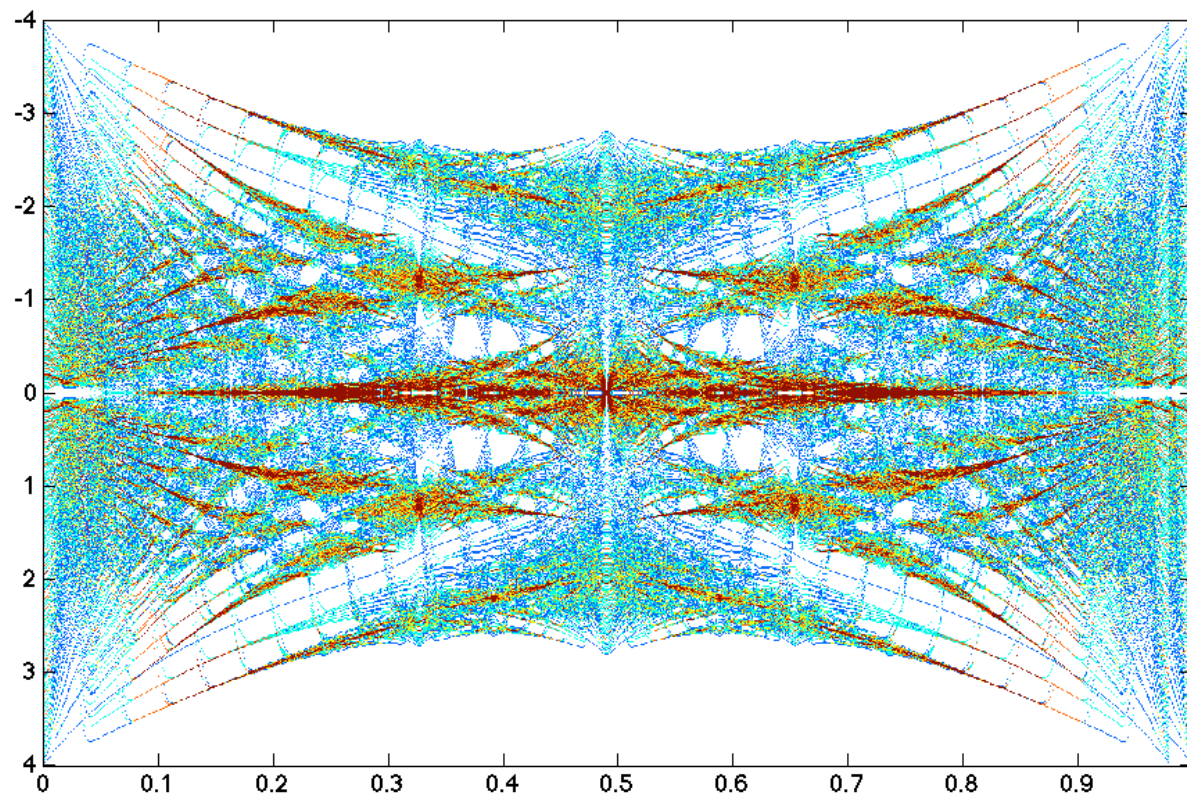
```



10×10

100 eigenvalues
50 parameter search

30×30
900 eigenvalues
900 parameter search



Single computation

$$\sim 132.88 \text{ sec} \times 900 \approx 33.22\text{h}$$

MPI computation

64 nodes  $\sim 2.7\text{h}$

Discussion

- MPI
 - Can use Libraries (Numerical Recipes,...)
 - Easy to use computing source(Nodes)
-
- CUDA
 - Need to remake Libraries (cuBLAS,...)
 - Need special source (GPU)