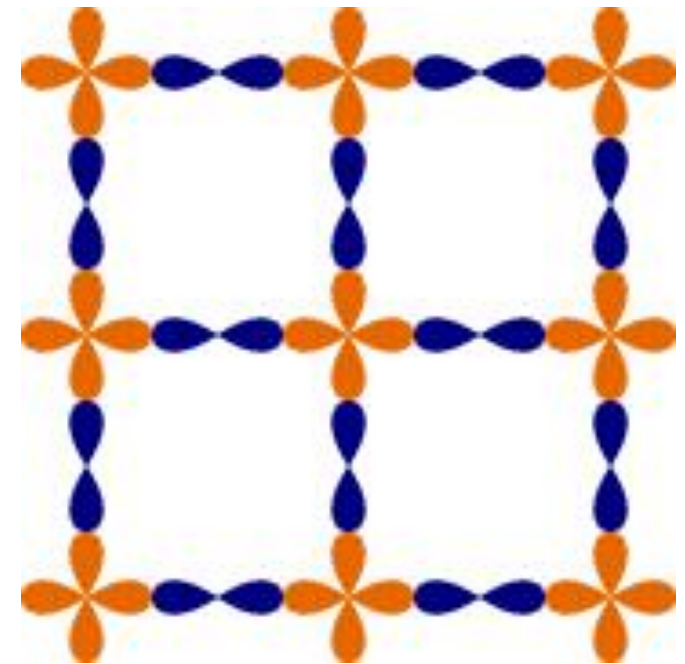


Discrete space (lattice) arises naturally in solids (crystals)

Using localized atomic-like orbitals (Wannier orbitals), called the **tight-binding method**, is often a good starting point for describing the electronic band structure

The hopping matrix elements can be obtained in band-structure calculations; can be non-zero also between non-nearest-neighbor sites

Tight-binding models form the basis of many calculations including also electron-electron and electron-phonon interactions



CuO_2 layers in the cuprate high- T_c superconductors

Lanczos diagonalization

Real-space discretized Hamiltonian is large in terms of $N \times N$

- but number of non-zero elements is $\sim N$, not N^2
- sparse matrix eigenvalue problem
- can use special methods for extremal eigenvalues/states

The Lanczos method is a **Krylov space method**

- space spanned by vectors $H^n |\Psi\rangle$

Idea: operate on expansion in energy eigenstates

$$H^m |\Psi\rangle = \sum_k C_k E_k^m |\Psi_k\rangle$$

For large m state with largest $|E_k|$ dominates the sum

- Acting multiple times with H projects out extremal state

Get ground state by acting with $(H - \sigma)^m$, $\sigma = \text{constant}$

- we will assume that a suitable constant has been included

Idea is to diagonalize H in space of all $H^n |\Psi\rangle$, $n = 0, \dots, m$

- can give low-lying states for small m (e.g., 100-500)

Lanczos basis states

Particular orthogonal basis of states $H^n|\Psi\rangle$, $n = 0, \dots, m$

➤ leads to a tridiagonal Hamiltonian matrix

➤ starts from arbitrary state $|\Psi\rangle$

First, orhogonal but not normalized basis $\{|f_n\rangle\}$

$|f_0\rangle$ arbitrary, normalized, overlap with $|\Psi_0\rangle$

$$|f_1\rangle = H|f_0\rangle - a_0|f_0\rangle$$

Chose constant such that the two states are orthogonal

$$\langle f_1|f_0\rangle = \langle f_0|H|f_0\rangle - a_0\langle f_0|f_0\rangle = H_{00} - a_0N_0$$

$$a_0 = H_{00}/N_0 \quad N_i = \langle f_i|f_i\rangle, \quad H_{ij} = \langle f_i|H|f_j\rangle$$

Next state; make it orthogonal to the two previous ones:

$$|f_2\rangle = H|f_1\rangle - a_1|f_1\rangle - b_0|f_0\rangle$$

$$a_1 = H_{11}/N_1, \quad b_0 = N_1/N_0$$

$$|f_{n+1}\rangle = H|f_n\rangle - a_n|f_n\rangle - b_{n-1}|f_{n-1}\rangle \quad H_{nn} = \langle f_n|H|f_n\rangle$$

$$a_n = H_{nn}/N_n, \quad b_{n-1} = N_n/N_{n-1} \quad N_n = \langle f_n|f_n\rangle$$

One can show that these states are orthogonal to all previous ones

Hamiltonian acting on a state

$$H|f_n\rangle = |f_{n+1}\rangle + a_n|f_n\rangle + b_{n-1}|f_{n-1}\rangle$$

This corresponds to a tri-diagonal matrix, non-zero elements are

$$\langle f_{n-1}|H|f_n\rangle = b_{n-1}N_{n-1} = N_n$$

$$\langle f_n|H|f_n\rangle = a_nN_n$$

$$\langle f_{n+1}|H|f_n\rangle = N_{n+1}$$

Normalized states $|\phi_n\rangle = N_n^{-1/2}|f_n\rangle$

$$\langle \phi_{n-1}|H|\phi_n\rangle = \sqrt{b_{n-1}}$$

$$\langle \phi_n|H|\phi_n\rangle = a_n$$

$$\langle \phi_{n+1}|H|\phi_n\rangle = \sqrt{b_n}$$

Algorithm for constructing the basis and the Hamiltonian

For the Hamiltonian, we need only the factors

$$a_n = H_{nn}/N_n, \quad b_0 = N_n/N_{n-1}$$

where $H_{nn} = \langle f_n | H | f_n \rangle$, $N_n = \langle f_n | f_n \rangle$

To obtain a new state we need the previous two:

$$|f_{n+1}\rangle = H|f_n\rangle - a_n|f_n\rangle - b_{n-1}|f_{n-1}\rangle$$

We have to store two states and the one we are working on.

$$|f_n\rangle = \sum_{j=1}^N f_n(j)|j\rangle \quad (\text{numbers } f_n(j), j=1, \dots, N \text{ stored})$$

We do not have to store H; act with it “on the fly”

$$V f_n(j)|j\rangle = V(j) f_n(j)|j\rangle \quad (V \text{ includes diag part of } K)$$

$$K f_n(j)|j\rangle = -t f_n(j) \sum_{\delta[j]} |\delta[j]\rangle, \quad \delta[j] \text{ neighbor of } j$$

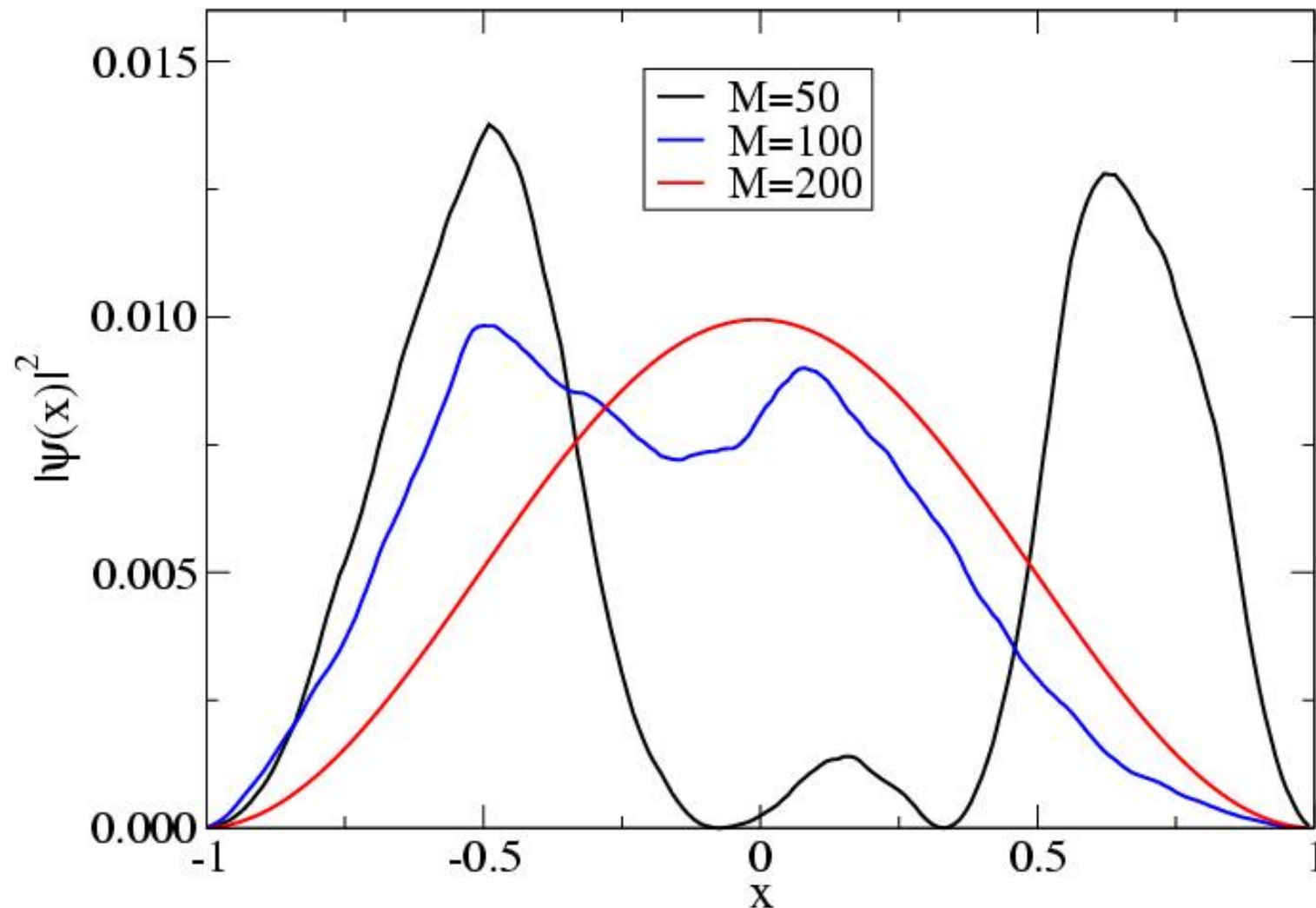
Need change in element index as particle “hops” between neighbors

1D test: Open chain (hard-wall box), $x=[-1,1]$ ($L=2$), $V=0$

Calculated energies as a function of Lanczos basis size M

N=200 $\Delta = 0.01$	10	165.47488	1116.18787	3077.75501
	20	36.464497	268.910471	744.48445
Very poor convergence	30	15.339143	155.724962	332.96633
	40	11.382975	86.779071	196.57548
	50	9.172055	47.562526	146.64266
	60	7.387181	27.980120	86.13795
	70	4.460574	16.659015	62.67232
Almost the full Hilbert space has to be included to get good energies	80	2.961753	14.353851	55.00397
	90	2.219407	13.280460	41.92692
	100	1.696802	12.229263	27.56645
	110	1.416573	11.376356	22.04370
	120	1.320332	10.941645	20.09118
	130	1.288321	10.732066	19.15900
	140	1.276327	10.613516	18.51138
	150	1.262146	10.191426	14.60174
	160	1.234164	6.045649	11.09876
	170	1.224724	5.160069	11.01756
Deviations at M=200 reflect discretization error (negative)	180	1.222428	4.974962	11.00148
	190	1.221635	4.905657	10.99395
	200	1.221430	4.885423	10.99108
	Exact	1.233701	4.934802	11.10330

Convergence of the ground state wave function



Lanczos method is not suitable for this type of calculation in 1D

➤ The basis must be of same size as the original one

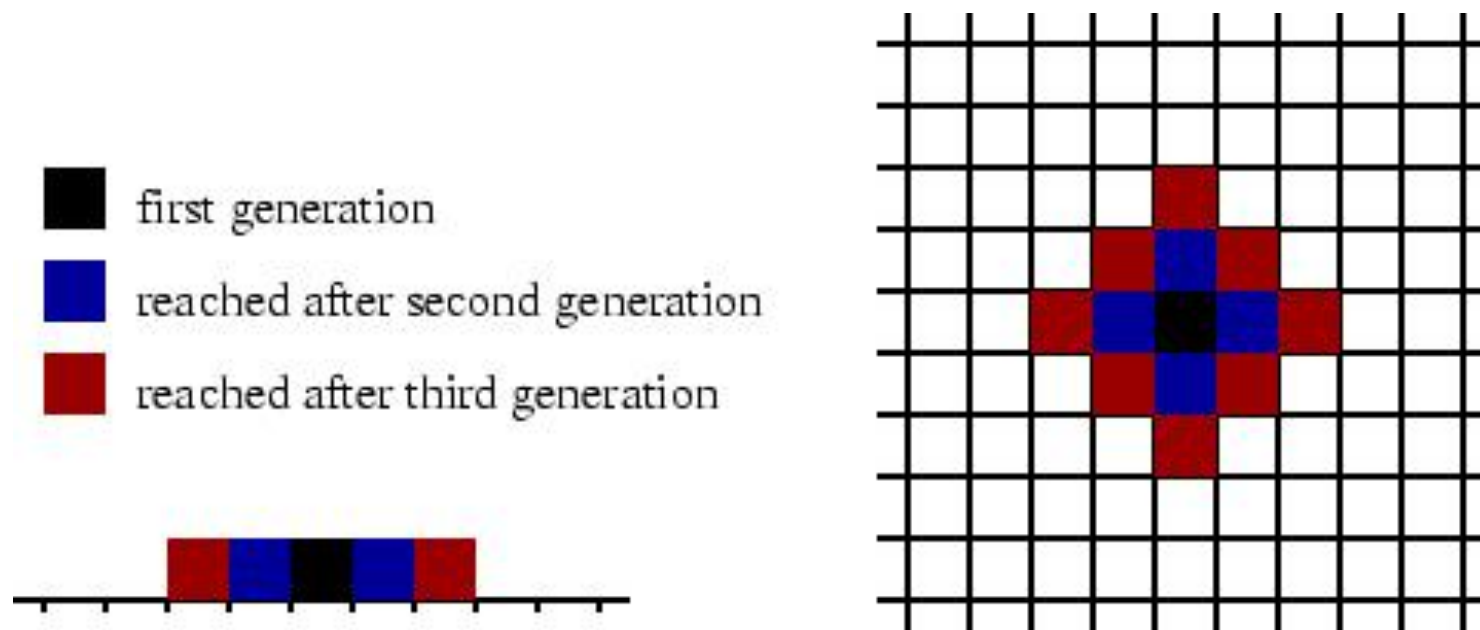
2D test: Open box (=hard-wall), $x,y=[-1,1]$, $V=0$

Energy as a function of Lanczos basis size M

N=200*200 $\Delta = 0.01$ Convergence after on the order of \sqrt{N} iterations	20	146.53700	731.057995	1807.662851
	40	36.89144	197.708305	466.352106
	60	19.78221	88.403669	216.571047
	80	14.33864	52.011927	120.846453
	100	11.36276	33.130912	78.125621
	120	9.836334	25.714048	59.319176
	140	9.093991	21.690312	43.007222
	160	8.460393	17.444110	31.878198
	180	7.719381	13.667132	26.425252
	200	6.494491	10.987755	22.538540
The method works better in 2D	240	5.310526	9.837896	18.969252
	280	3.925524	7.766020	11.142274
	320	2.815453	6.526244	10.305297
	360	2.482839	6.177734	9.963101
	400	2.447032	6.119496	9.841073
	440	2.443210	6.108594	9.789598
	480	2.442875	6.106960	9.772831
	Exact	2.467401	6.168503	9.869604

The components (i.e., individual basis states) of the initial state must be propagated by the Hamiltonian through the whole system in order for an extended wave function to be representable in the Lanczos basis

Regions covered after successive operations with H (“generations”) on a single basis state in 1D and 2D



Covered fraction scales as the number of generations M in any D

➤ The Lanczos scheme is advantageous in 2D and 3D