The Schrodinger equation in discretized real space

Example of grid-based method for 2D and 3D problems

Basis of states localized in small volume element

➢ large number of such states neded in 2D and 3D

➢ the resulting N*N matrix is too big to be fully diagonalized

➢ special methods exist for lowest states of sparse matrices

- N up to several million (even 10s or 100s of millions)

Cubic d-dimensional space elements;

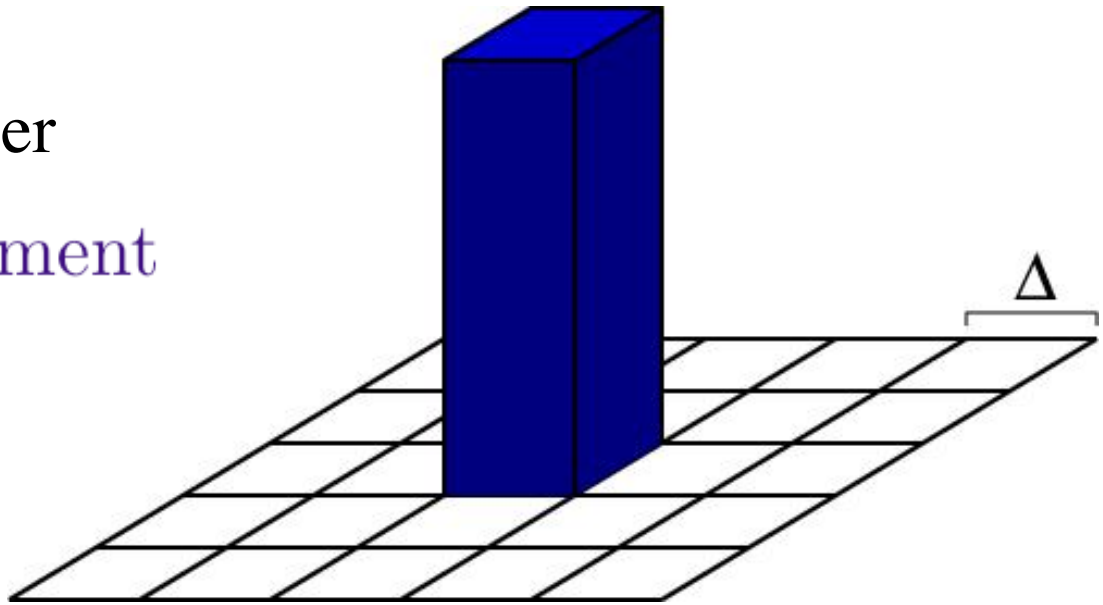
$$\text{volume} = \Delta^d$$

Label by coordinate or number

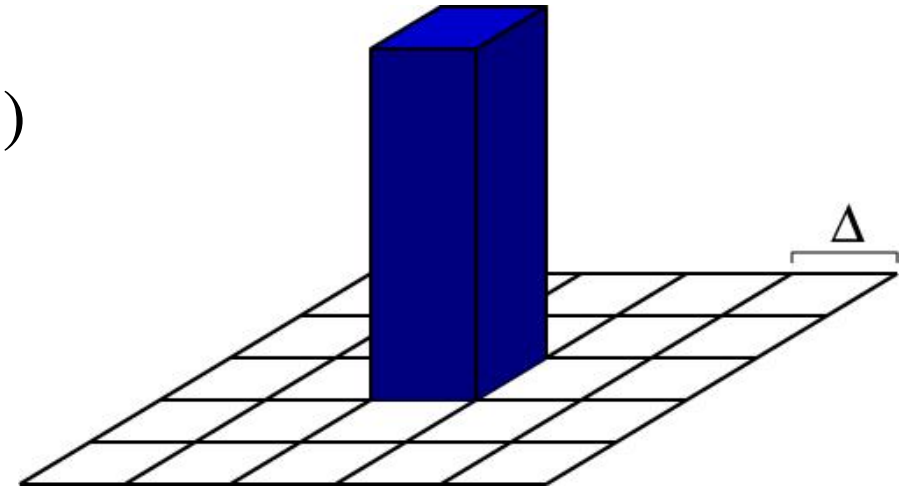
$$\phi_j(\vec{x}) = \frac{1}{\Delta^{d/2}} \quad \text{inside element}$$

Coordinate of element $\vec{r}_j$

Non-overlapping $\langle j|l\rangle = \delta_{jl}$
(orthonormal basis)



Strictly speaking, these are not valid wave functions (discontinuous)



However, we will obtain a scheme that gives the correct physics in the limit $\Delta \to 0$

(we could also in principle use some continuous localized functions)

Size of the basis in a box with side L: $N = (L/\Delta)^d$

Matrix elements of Hamiltonian $H = K + V$

The potential energy is diagonal

$$V_{jl} = \langle j|V|l\rangle = \delta_{jl} \int dx^d |\phi_j(\vec{x})|^2 V(\vec{x}) \approx \delta_{jl} V(\vec{r}_j)$$

Kinetic energy

$$K_{jl} = \langle j|K|l\rangle = \frac{-1}{2} \int dx^d \phi_j^*(\vec{x}) \nabla^2 \phi_l(\vec{x})$$

How do we deal with the non-differentiability?

Using central difference operator in place of derivatives

➢ Can we do this when the functions are not smooth?

➢ We will show that it in fact produces correct results

Work in one dimension for simplicity

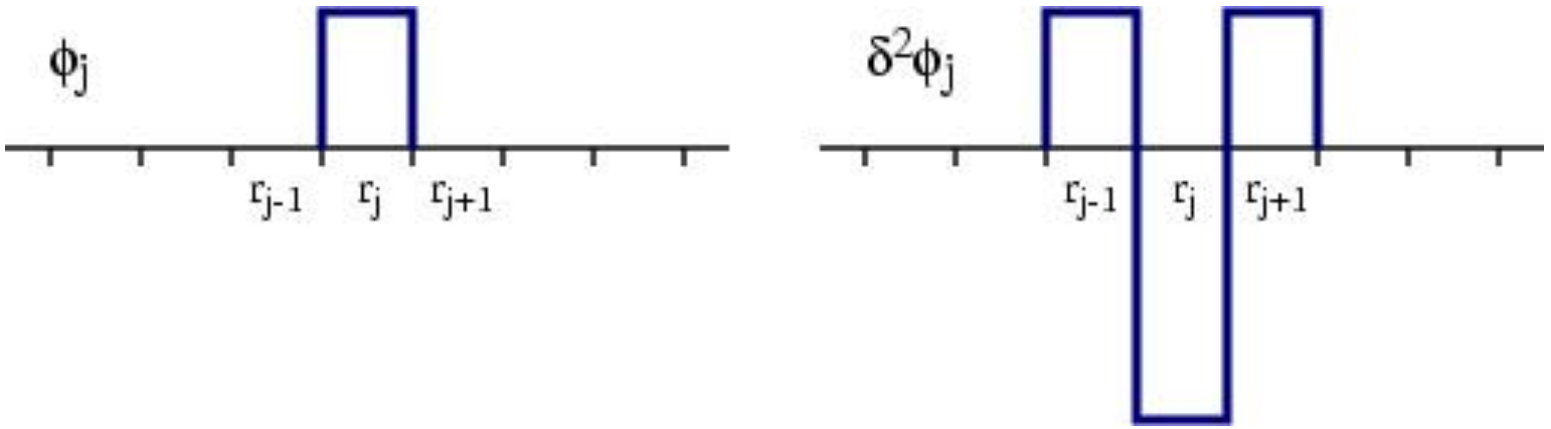
- Can be directly generalized to higher dimensionality

Replace second derivatives of the basis functions by

$$\frac{1}{\Delta^2}\delta^2\phi_j(x) = \frac{1}{\Delta^2}[\phi_j(x-\Delta) - 2\phi_j(x) + \phi_j(x+\Delta)]$$

$$= \frac{1}{\Delta^2}[\phi_{j-1}(x) - 2\phi_j(x) + \phi_{j+1}(x)]$$

Produces non-zero values in the neighboring elements



The kinetic energy matrix elements are

$$K_{jl} = -\frac{1}{2}\int dx^d \phi_j^*(\vec{x})\frac{1}{\Delta^2}\delta^2\phi_l(\vec{x}) = \begin{cases} -\Delta^{-2}/2, & \text{for } j = l \pm 1 \\ \Delta^{-2}, & \text{for } j = l \end{cases}.$$

This means that when K acts on a state

$$K|j\rangle = -\frac{1}{\Delta^2}\left[\frac{1}{2}|j-1\rangle - |j\rangle + \frac{1}{2}|j+1\rangle\right]$$

Non-zero matrix elements of the full Hamiltonian

$$H_{j,j} = V(r_j) + \frac{1}{\Delta^2} \qquad H_{j\pm1,j} = -\frac{1}{2}\frac{1}{\Delta^2}$$

Generalizes to 2D and 3D; kinetic energy "hops" localized particle between nearest-neighbor volume elements

$$H_{j,j} = V(\vec{r}_j) + \frac{d}{\Delta^2} \qquad H_{\delta[j],j} = -\frac{1}{2}\frac{1}{\Delta^2}$$

$\delta[j]$ denotes a neighbor of j (2,4,6 neighbors in 1D, 2D, 3D)

Proof of correct continuum limit for free particle in a box

1D for simplicity (generalizes easily)

Periodic box of length L; energy eigenstates

$$\phi_k(x) = \mathrm{e}^{-ikx}, \quad \text{with} \quad k = n2\pi/L, \quad n = 0, 1, \ldots$$

Energy: $E_k = \frac{1}{2}k^2 \quad (\hbar = m = 1)$

Discretized space, N cells; we will prove that the eigenstates are

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \mathrm{e}^{-ikr_j} |j\rangle, \quad k = n2\pi/L \quad \text{with} \quad n = 0, 1, \ldots, N-1$$

Discrete coordinate $r_j = j\Delta = jL/N$ limits momentum;

$$\mathrm{e}^{-i(n+N)2(\pi/L)r_j} = \mathrm{e}^{-in2(\pi/L)r_j}$$

so only N different momenta

Acting with kinetic energy on proposed state:

$$K|k\rangle = -\frac{1}{\Delta^2}\frac{1}{\sqrt{N}}\sum_{j=0}^{N} \mathrm{e}^{-ikr_j}\left[\frac{1}{2}|j-1\rangle - |j\rangle + \frac{1}{2}|j+1\rangle\right]$$

Shifting the indexes in the j +/- 1 terms by +/- 1

$$K|k\rangle = -\frac{1}{\Delta^2}\frac{1}{\sqrt{N}}\sum_{j=0}^{N} \mathrm{e}^{-ikr_j}\left[\frac{1}{2}(\mathrm{e}^{ik\Delta} + \mathrm{e}^{-ik\Delta}) - 1\right]|j\rangle$$

$$= \frac{1}{\Delta^2}[\cos(k\Delta) - 1]|k\rangle$$

Energy eigenvalues are $E_k = \frac{1}{\Delta^2}[1 - \cos(k\Delta)]$

Taylor expand for small $k\Delta$

$$E_k = \frac{1}{2}k^2 - \frac{1}{24}\Delta^2 k^4 + \ldots$$

Agrees with continuum result to leading order, i.e., the way we treated the kinetic energy in the discretized space was ok.

Note that the discretized energy is lower than the true energy

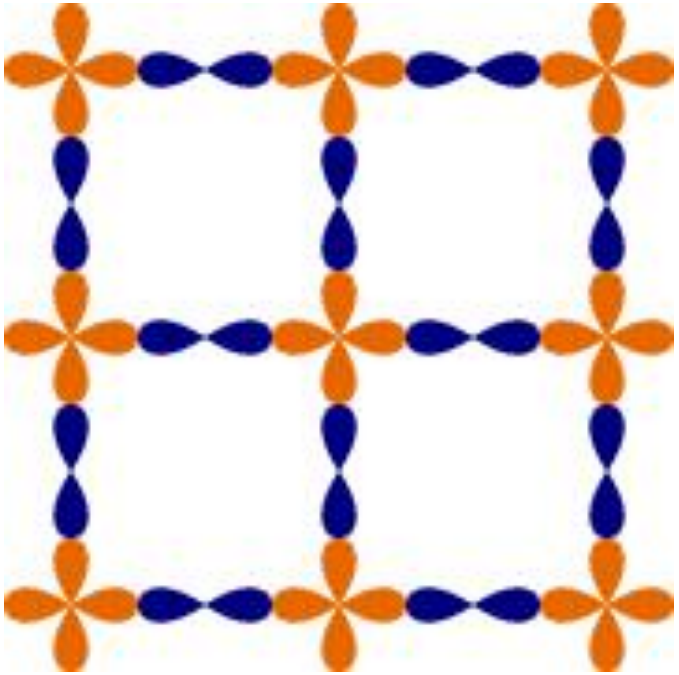
3D: $E_k = \frac{1}{\Delta^2}[3 - \cos(k_x\Delta) - \cos(k_y\Delta) - \cos(k_z\Delta)]$

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*N

➢ but number of non-zero elements is ~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 $(H-\sigma)^m, \quad \sigma = \text{constant}$

➢ we will assume that a suitable constant has been included

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

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

Lanczos basis states

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

➢ 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

$$\langle f_1|f_0\rangle = \langle f_0|H|f_0\rangle - a_0\langle f_0|f_0\rangle = H_{00} - a_0 N_0$$

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

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

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

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

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

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

$$N_n = \langle f_n|f_n\rangle$$

$$a_n = H_{nn}/N_n, \qquad b_{n-1} = N_n/N_{n-1}$$

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

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

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

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

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

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.

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

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

$$V f_n(j)|j\rangle = V(j) f_n(j)|j\rangle$$ (V 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 neigbors

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

$\Delta = 0.01$

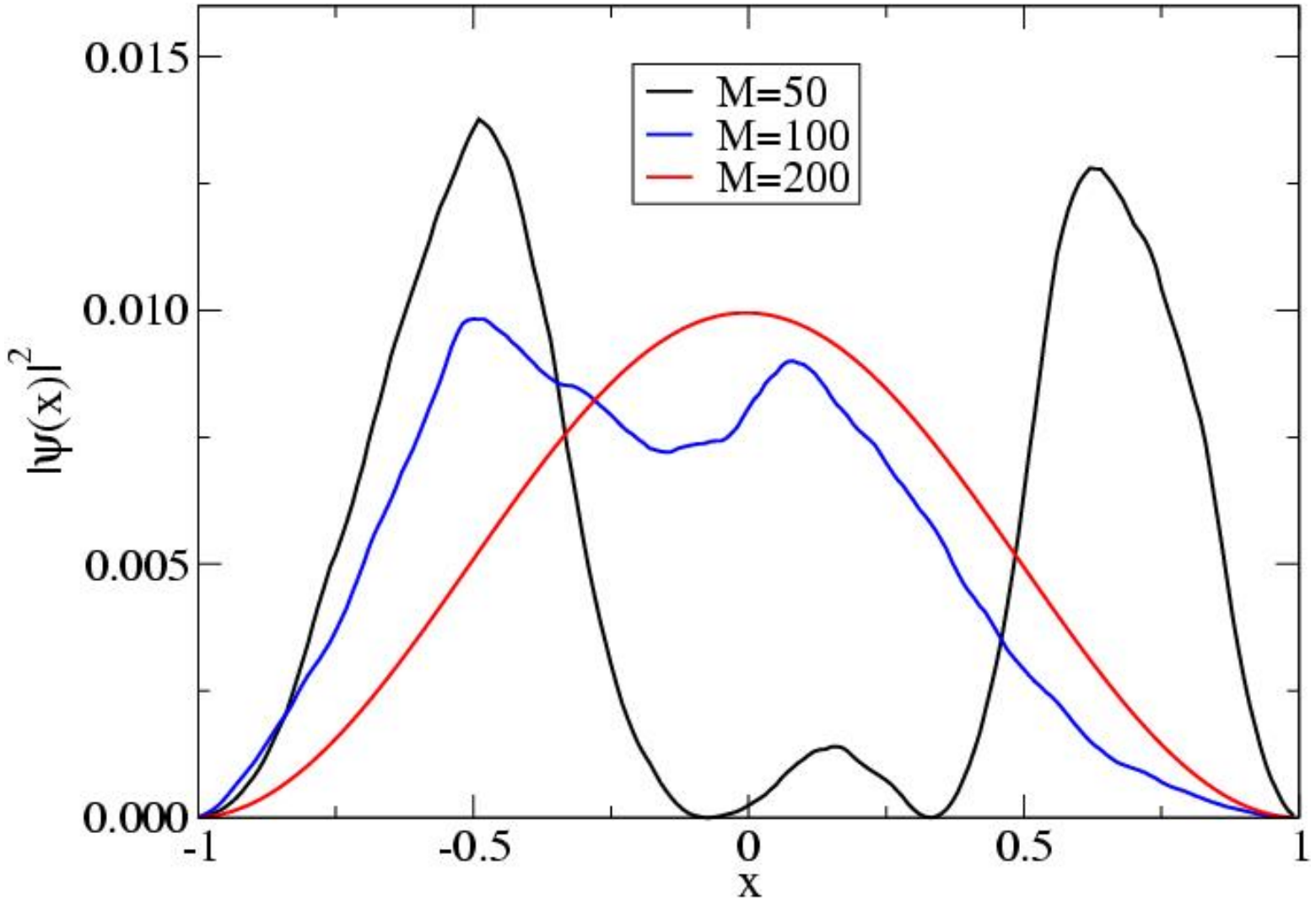
Very poor convergence

Almost the full Hilbert space has to be included to get good energies

Deviations at M=200 reflect discretization error (negative)

10	165.47488	1116.18787	3077.75501
20	36.464497	268.910471	744.48445
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
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
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

The method works better in 2D

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
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