The Schrödinger 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 needed in 2D and 3D
- the resulting $N \times N$ 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;
volume $= \Delta^d$

Label by coordinate or number

$\phi_j(\bar{x}) = \frac{1}{\Delta^{d/2}}$ 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

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

Kinetic energy

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

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

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
\[ H_{j,j} = V(r_j) + \frac{1}{\Delta^2} \quad H_{j\pm1,j} = -\frac{1}{2} \frac{1}{\Delta^2} \]

Generalizes to 2D and 3D; kinetic energy “hops” localized particle between nearest-neighbor volume elements
\[ H_{j,j} = V(\mathbf{r}_j) + \frac{d}{\Delta^2} \quad H_{\delta[j],j} = -\frac{1}{2} \frac{1}{\Delta^2} \]

\( \delta[j] \) 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

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

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

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

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

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

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

so only $N$ different momenta
Acting with kinetic energy on proposed state:

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

Shifting the indexes in the \( j +/\- 1 \) terms by +/- 1

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

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

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 $N^2$ 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 $H^n |\Psi\rangle$, $n = 0, \ldots, m$

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

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

- leads to a tridiagonal Hamiltonian matrix
- starts from arbitrary state $|\Psi\rangle$

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

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

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

Choose 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:

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

$a_1 = H_{11}/N_1 \quad b_0 = N_1/N_0$
\[ |f_{n+1}\rangle = H |f_n\rangle - a_n |f_n\rangle - b_{n-1} |f_{n-1}\rangle \]
\[ H_{nn} = \langle f_n | H | f_n \rangle \]
\[ a_n = H_{nn} / N_n, \quad b_{n-1} = N_n / N_{n-1} \]
\[ N_n = \langle f_n | f_n \rangle \]

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

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

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

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.

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

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

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

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

Need change in element index as particle “hops” between neighbors
### Calculated energies as a function of Lanczos basis size $M$

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<th>$M$</th>
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<th>$E_1$ (negative)</th>
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Deviations at $M=200$ reflect discretization error (negative)
The Lanczos method is not suitable for this type of calculation in 1D. The basis must be of the same size as the original one.