QM point-particle in external potential (part 1) – v1

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Contents

1 Goals for subproject 2

The following essential modules, main programs and test programs need to be coded. *Important: The notation is explained in the subsequent sections.*

Hamiltonian module. This module needs to contain (at least) three functions:

1. a function that calculates the dimensionless potential (we are considering only the quartic potential described in the notes);

2. the kinetic energy function, which takes $\hat{\psi}$ and returns $\hat{H}_a\hat{\psi}$ for the particular case $V = 0$;
3. the Hamiltonian function, which takes $\hat{\psi}$ and returns $\hat{H}_a\hat{\psi}$; this function must use the ones defined in the previous points.

Only dimensionless parameters must appear in the code. The Hamiltonian depends on N, μ, ϵ^2. All these parameters should be treated as global variables. The code should be written to work in a generic number of dimensions D. If you work in Python/Julia, you may want to represent discretized wave functions as D-dimensional arrays. If you work in C/C++, you will need to flatten the array (talk to me about this).

Eigenvalues/eigenvector module. This module contains three functions.

1. The first function implements the power method, with the specifications given in the warm-up exercise.
2. The second function implements the conjugate gradient, with the specifications given in the warm-up exercise.
3. The third function calculates the smallest eigenvalue of A and the corresponding eigenvector, using the previous two functions. Input:
   - function $v \mapsto Av$ (you must pass a function, and not the matrix A);
   - tolerance of the power method;
   - maximum number of iterations of the power method.
   - tolerance of the conjugate gradient;
   - maximum number of iterations of the conjugate gradient.

   Output:
   - Eigenvalue and eigenvector.

The code needs to be general enough to be able to take functions $v \mapsto Av$ that act on wavefunctions.

Observable module. This module contains several functions. Each of them takes a wavefunction as input and returns one observable. The following observables need to be considered:

1. expectation value of the energy,
2. expectation value of the position,
3. expectation value of the momentum,
4. indetermination of the position,
5. indetermination of the momentum,
6. probability to find the particle in the half-line $x > 0$.

Ground-state main program. You should write a program that

1. reads the relevant parameters from an input file or from command line,
2. calculates the lowest eigenvalue and eigenvector of the Hamiltonian given in the notes using the modules defined above,
3. writes the eigenvector to file (so that the wavefunction can be plotted at a later time),
4. calculates and prints all observables defined in the observable module.

Test programs. The following test programs need to be coded, run, and described in a short report. The outcome of the tests need to be described as well. Remember: the aim of a test program is to convince yourself and us that the code is correct.

- After solving the exercises proposed in section 5, write programs that test the linearity, hermiticity and positivity of the Hamiltonian operator. Write a program that tests that the eigenvalues and eigenvector of the kinetic energy operator are the ones found in section 5.
- Incorporate (and re-run) the tests for the power method and the conjugate gradient given in the warm-up exercise.

Run the program with $D = 1$, $N = 200$, $\mu = 20$, $\epsilon^2 = 0.001$ and present the results. Change the parameters, and try to extrapolate to the infinite-volume limit (i.e. $L \to \infty$) and to the continuum limit (i.e. $a \to 0$). Discuss your extrapolations in the report.

Run the program with $D = 2$, $N = 200$, $\mu = 20$, $\epsilon^2 = 0.001$, critically interpret and present the results.

2 Problem

The quantum mechanical point particle in D dimensions in external potential is described by the following Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \ . \tag{1}$$

In Quantum Mechanics, the position $\mathbf{x}$, the momentum $\mathbf{p}$ and the Hamiltonian H are linear operators acting on the space of states of the system (Hilbert space). Position and momentum operators satisfy the canonical commutation relation

$$[x_j, p_k] = i\hbar\delta_{ij} \ . \tag{2}$$

The states of the point particle can be identified with the wavefunctions $\psi(\mathbf{x})$. Assuming that the wavefuction is normalized, i.e.

$$\int d^D x \, |\psi(\mathbf{x})|^2 = 1 \ , \tag{3}$$

then $|\psi(\mathbf{x})|^2$ is the probability density that the particle is in $\mathbf{x}$, i.e. $|\psi(\mathbf{x})|^2 d^D x$ is the probability that the particle is in an infinitesimal volume $d^D x$ centered in $\mathbf{x}$. The position operator acts as a multiplication operator

$$\psi(\mathbf{x}) \overset{\mathbf{x}}{\mapsto} \mathbf{x}\psi(\mathbf{x}) \ , \tag{4}$$

while the momentum operator is proportional to the gradient, i.e.

$$\psi(\mathbf{x}) \overset{\mathbf{p}}{\mapsto} -i\hbar\nabla\psi(\mathbf{x}) \ . \tag{5}$$

Putting everything together, one finds that the Hamiltonian acts of wavefunctions as

$$H\psi(\mathbf{x}) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x}) \ . \tag{6}$$

The state with wavefunction $\psi(\mathbf{x})$ can be equivalently described by the wavefuncion in momentum space, i.e.

$$\tilde{\psi}(\mathbf{p}) = \int \frac{d^3 p}{(2\pi)^3} e^{-\frac{i}{\hbar}\mathbf{p}\mathbf{x}} \psi(\mathbf{x}) \ . \tag{7}$$

Assuming normalization

$$\int \frac{d^3 p}{(2\pi)^3} \, |\tilde{\psi}(\mathbf{p})|^2 = 1 \ , \tag{8}$$

$|\tilde{\psi}(\mathbf{p})|^2 \frac{d^3 p}{(2\pi)^3}$ is the probability that the particle has a momentum inside an infinitesimal volume $d^D p$ centered in $\mathbf{p}$.

The *time-independent Schrödinger equation*

$$H\psi_n = E_n \psi_n \tag{9}$$

is nothing but the eigenvalue equation for the Hamiltonian. The eigenvectors ψ_n are also called eigenfunctions or eigenstates or stationary states, and the eigenvalues E_n are called energy levels. The eigenstate corresponding to the smallest energy level is also called ground state.

The time evolution of states is governed by the *time-dependent Schrödinger equation*

$$i\frac{\partial}{\partial t}\psi_t = H\psi_t \ . \tag{10}$$

Given an initial condition ψ_0, the solution of this equation is formally written by means of the exponential function, i.e.

$$\psi_t = e^{-\frac{i}{\hbar}Ht}\psi_0 \ . \tag{11}$$

In this project we will consider the potential

$$V(\mathbf{x}) = \frac{m\omega^2}{8r^2}(\mathbf{x}^2 - r^2)^2 \ . \tag{12}$$

Plot this potential, and study its features.

There are two important steps to take, in order to be able to represent this system on the computer: discretize the system, and express all interesting observables in terms of dimensionless parameters. We will discuss these two steps in the next two sections.

3 Lattice discretization

One needs to observe that the wavefunction $\psi(\mathbf{x})$ cannot be represented exactly on a computer, since you would need to store a complex number for each of the infinitely-many points $\mathbf{x} \in \mathbb{R}^D$.

In order to circumvent this problem, we replace the continuous infinite space $\mathbb{R}^D$ with a finite regular lattice (or grid, or crystal), with a lattice spacing a and N points in each direction. This means that the coordinates $\mathbf{x}$ can only take values of the type

$$x_k = an_k \ , \quad \text{with } n_k = 0, 1, 2, \ldots, N-1 \ , \tag{13}$$

or alternatively

$$x_k = an_k \ , \quad \text{with } n_k = \begin{cases} -\frac{N}{2}+1, \ldots, 0, \ldots, \frac{N}{2} & \text{if } N \text{ even} \\ -\frac{N-1}{2}, \ldots, 0, \ldots, \frac{N-1}{2} & \text{if } N \text{ odd} \end{cases} \ . \tag{14}$$

Notice that in all cases one has exactly N possible values for n_k. In some cases it may be even convenient to consider the case in which n_k is half-integer. On case of external potential, the problem is clearly not translational invariant, therefore these choices are not equivalent. For instance, in the case of a central potential, the center of the potential should be located in the center of the lattice. Therefore one could keep the center in the origin with the choice (14), but the center should be in $\mathbf{n} = (N/2, N/2, \ldots, N/2)$ with the choice (13).

The linear size of the lattice is given by $L = Na$, and its volume by L^D. Notice that the lattice has now a total number of point N^D which is finite. Therefore, in order to specify the wavefunction, one only needs to specify N^D complex numbers. In your code, these numbers may be organized in a D-dimensional array or in a 1-dimensional array (using e.g. a lexicographic index): either choice is equally acceptable.

In the continuum the normalization condition involves an integral over the space. When the space is replaced with a lattice, one can approximate the integral with a Riemann sum, i.e.

$$\int d^D x \to \sum_{\mathbf{x}} a^D \ . \tag{15}$$

Notice that the integral is not replaced just by the sum, but you must include the volume of the smallest cell a^D. Therefore the normalization condition reads

$$\sum_{\mathbf{x}} a^D |\psi(\mathbf{x})|^2 = 1 \ . \tag{16}$$

In order to understand how the Hamiltonian acts on discretized wavefunction, we need to look at the Laplacian. We notice that, in the continuum,

$$\nabla^2 \psi(\mathbf{x}) = \sum_k \frac{\partial^2}{\partial x_k^2} \psi(\mathbf{x}) = \lim_{a \to 0} \sum_k \frac{\psi(\mathbf{x} + a\mathbf{e}_k) + \psi(\mathbf{x} - a\mathbf{e}_k) - 2\psi(\mathbf{x})}{a^2} \ , \tag{17}$$

where $\mathbf{e}_k$ is the unit vector in the direction k. This formula can be easily proved e.g. by using de l'Hôpital twice (try it!). Then the discretized version of the Laplacian can be simply defined by dropping the limit. Therefore the discretized Hamiltonian can be chosen to be

$$H_a \psi(\mathbf{x}) = -\frac{\hbar^2}{2ma^2} \sum_k [\psi(\mathbf{x} + a\mathbf{e}_k) + \psi(\mathbf{x} - a\mathbf{e}_k) - 2\psi(\mathbf{x})] + V(\mathbf{x})\psi(\mathbf{x}) \ . \tag{18}$$

Notice that the discretized Laplacian in $\mathbf{n}$ is constructed by means of the nearest neighbouring points of $\mathbf{n}$. On a finite lattice, points at the boundary do not have nearest neighbours in all directions. In this case, boundary conditions must be provided to make sense of eq. (18) at the boundary. **You are required to use periodic boundary conditions.**

4 Units of measure

Let's say that you have an energy of $E = 1$ J and you want to represent this in your computer. It is tempting to use a variable $E = 1$, and you need to remember that energies in your code are meant to be in Joules. The computer does not really understand units of measure, in fact the information that E needs to be interpreted in Joules needs to be stored somewhere else (e.g. in your brain, or in a note). At any point, you may also decide to use a different unit system. For instance your energy is also equal to $E \simeq 6 \times 10^{18}$ eV. So, an equally good choice would be to store $E = 6 \times 10^{18}$. Why would you prefer $E = 1$ over $E = 6 \times 10^{18}$? If you think about it, there is really no reason.

The point is that unit systems are quite arbitrary, but the physics does not depend on the choice of unit systems. If one chooses to measure energies, lengths... in terms of intrinsic scales of the problem rather than in units of an arbitrarily-chosen unit system, then one can express the problem entirely in terms of dimensionless quantities. These dimensionless quantities can then naturally be used in variables in your code, avoiding any ambiguity due to the choice of unit system. Let's see how this works in our case.

Let us look at the Hamiltonian of the continuous system first

$$H = -\frac{\hbar^2}{2m} \nabla^2 + \frac{m\omega^2}{8r^2} (\mathbf{x}^2 - r^2)^2 \ , \tag{19}$$

which depends on the parameters m, $\hbar$, ω, r. The units of the parameters are easily extracted by means of dimensional analysis

$$[\hbar] = \text{mass} \times \text{length}^2 \times \text{time}^{-1} \ , \tag{20}$$

$$[r] = \text{length} \ , \tag{21}$$

$$[m] = \text{mass} \ , \tag{22}$$

$$[\omega] = \text{time}^{-1} \ , \tag{23}$$

$$[H] = \text{energy} = \text{mass} \times \text{length}^2 \times \text{time}^{-2} \ . \tag{24}$$

There are two natural energy scales in this problem. The first one is $\hbar\omega$ which is the energy gap associated to the small oscillations around the minima of the potential (in this regime the system is approximated by a harmonic oscillator). The second one is the energy barrier $\Delta V = V(0) - V(r) = \frac{1}{8} m\omega^2 r^2$.

Rather than measuring energies in Joules or in eV, we decide to measure energies in units of $\hbar\omega$ (but using the other energy scale would be equally acceptable). The Hamiltonian in units of $\hbar\omega$ is a dimensionless operator, which we will denote by

$$\hat{H} = \frac{H}{\hbar\omega} = -\frac{\hbar}{2m\omega}\nabla^2 + \frac{m\omega}{8\hbar r^2}(\mathbf{x}^2 - r^2) = -\frac{\hbar}{2m\omega r^2}\sum_k r^2 \frac{\partial^2}{\partial x_k^2} + \frac{m\omega r^2}{8\hbar}\left(\frac{\mathbf{x}^2}{r^2} - 1\right)^2 \ . \tag{25}$$

Notice that the coefficients in terms of the dimesionless operator $r^2\nabla^2$ and the dimensionless combination $\left(\frac{\mathbf{x}^2}{r^2} - 1\right)^2$ are both dimensionless and they are trivially related to each other. Therefore we introduce the dimensionless parameter

$$\mu = \frac{m\omega r^2}{\hbar} \ , \tag{26}$$

in terms of which the Hamiltonian in units of $\hbar\omega$ is

$$\hat{H} = \frac{H}{\hbar\omega} = -\frac{1}{2\mu}\sum_k r^2 \frac{\partial^2}{\partial x_k^2} + \frac{\mu}{8}\left(\frac{\mathbf{x}^2}{r^2} - 1\right)^2 \ . \tag{27}$$

This formula suggests to measure all distances in units of the intrinsic scale r, and this would be indeed the most natural course of action in the continuum. However, in the case of the discretized theory, it is more natural to measure distances in units of the lattice spacing a. In fact we have already introduced the position vector in units of the lattice spacing, i.e.

$$\mathbf{n} = \frac{\mathbf{x}}{a} \ . \tag{28}$$

Before looking at the discretized Hamiltonian, let us look at the discretized wavefunction. Notice that the normalization condition

$$\sum_{\mathbf{x}} a^D |\psi(\mathbf{x})|^2 = 1 \tag{29}$$

implies that the wavefunction as dimension $\text{length}^{-D/2}$, therefore we can introduce the wavefunctions in units of $a^{-D/2}$, i.e.

$$\hat{\psi}(\mathbf{n}) = \frac{\psi(a\mathbf{x})}{a^{-D/2}} = a^{D/2}\psi(a\mathbf{x}) \ . \tag{30}$$

The normalization condition for the dimensionless wavefunction reads simply

$$\sum_{\mathbf{n}} |\hat{\psi}(\mathbf{n})|^2 = 1 \ . \tag{31}$$

Starting from eqs. (18) and (27), we are now ready to write the action of the discretized Hamiltonian in units of $\hbar\omega$ on the dimensionless wavefunction, i.e.

$$\hat{H}_a\hat{\psi}(\mathbf{n}) = \frac{H_a}{\hbar\omega}\hat{\psi}(\mathbf{n}) = -\frac{1}{2\mu}\frac{r^2}{a^2}\sum_k [\hat{\psi}(\mathbf{n}+\mathbf{e}_k) + \hat{\psi}(\mathbf{n}-\mathbf{e}_k) - 2\psi(\mathbf{n})] + \frac{\mu}{8}\left(\frac{a^2}{r^2}\mathbf{n}^2 - 1\right)^2 \hat{\psi}(\mathbf{n}) \ . \tag{32}$$

Finally, we introduce the dimensionless parameter

$$\epsilon = \frac{a}{r} \tag{33}$$

and we write the discretized Hamilonian in units of $\hbar\omega$ entirely in terms of dimesionless parameters

$$\hat{H}_a\hat{\psi}(\mathbf{n}) = -\frac{1}{2\mu\epsilon^2}\sum_k [\hat{\psi}(\mathbf{n}+\mathbf{e}_k) + \hat{\psi}(\mathbf{n}-\mathbf{e}_k) - 2\psi(\mathbf{n})] + \frac{\mu}{8}\left(\epsilon^2\mathbf{n}^2 - 1\right)^2 \hat{\psi}(\mathbf{n}) \ . \tag{34}$$

Notice that in the original formulation (19) the Hamiltonian depends of 4 parameters $\hbar$, m, ω r. After discretization we also introduce the lattice spacing a and the lattice extent L, for a total of 6 dimensionful parameters. However, in the formulation (34), the discretized Hamiltonian depends only on 3 dimensionless parameters: μ, ϵ and $N = L/a$. The second formulation has two important advantages: it is is more economical (i.e. it avoids redundances), and it does not depend on the arbitrariness of the choice of unit system. **You must use the second approach in your code, i.e. only dimensionless parameters must appear in your code.**

5 Tests of Hamiltonian

Solve the following problems (the solutions should be written down in the report). Each problem can be used to design a test program for the Hamiltonian.

Linearity. Prove that

$$\hat{H}_a(\alpha\hat{\psi} + \beta\hat{\phi}) = \alpha(\hat{H}_a\hat{\psi}) + \beta(\hat{H}_a\hat{\phi}) \tag{35}$$

for any complex numbers α, β, and any wavefunctions $\hat{\psi}, \hat{\phi}$.

Write a program that tests this property.

Hermiticity. Prove that

$$\left(\hat{\psi}, \hat{H}_a\hat{\phi}\right) = \left(\hat{H}_a\hat{\psi}, \hat{\phi}\right) \tag{36}$$

for any wavefunctions $\hat{\psi}, \hat{\phi}$. Here the scalar product is defined as:

$$\left(\hat{\psi}, \hat{\phi}\right) = \sum_{\mathbf{n}} \hat{\psi}(\mathbf{n})^* \hat{\phi}(\mathbf{n}) \ . \tag{37}$$

Write a program that tests this property.

Positivity. Prove that, if $V \geq 0$, then

$$\left(\hat{\psi}, \hat{H}_a \hat{\psi}\right) \geq 0 \tag{38}$$

for any wavefunction $\hat{\psi}$.

Write a program that tests this property.

Eigenvalues and eigenvectors. Prove that, if $V = 0$, then the plane waves

$$\hat{\psi}_{\mathbf{k}}(\mathbf{n}) = e^{\frac{2\pi i \mathbf{n}\mathbf{k}}{N}} , \qquad \mathbf{k} \in \mathbb{Z}^D \tag{39}$$

are eigenfunctions of $\hat{H}_a$ (with periodic boundary conditions) and calculate the corresponding eigenvalue $E_{\mathbf{k}}$.

Write a program that checks that eigenvalue equation $\hat{H}_a \hat{\psi}_{\mathbf{k}} = E_{\mathbf{k}} \hat{\psi}_{\mathbf{k}}$ is satisfied.

6 Numerical calculation of the ground state

We want to calculate the ground state of $\hat{H}_a$, i.e. the eigenvector associated to the smallest eigenvalue of $\hat{H}_a$. We are going to combine two algorithms to do this: the power method, and the conjugate gradient.

6.1 Power method

Given a positive semidefinite square matrix A, the power method allows to calculate an approximation of the largest eigenvalue of A and of the corresponding eigenvector. It is based on the following theorem.

Theorem. Given a positive semidefinite square matrix A and a vector z, construct

$$v = \lim_{n \to \infty} \frac{A^n z}{\|A^n z\|} . \tag{40}$$

For almost every z, the above limit exits and v is an eigenvector of A associated to its largest eigenvalue.

Proof. Let $\lambda_1 > \lambda_2 > \cdots > \lambda_M (\geq 0)$ be the eigenvalues of A. Let d_i be the degeneracy do the eigenvalue λ_i. Let w_{ip} be eigenvectors corresponding to the eigenvalue λ_i, where the index $p = 1, \ldots, d_i$ distinguishes between degenerate eigenvectors. We choose the eigenvectors to form an orthonormal basis, i.e.

$$w_{ip}^\dagger w_{jq} = \delta_{ij} \delta_{pq} . \tag{41}$$

Then we can decompose the vector z with respect to the basis given by the eigenvectors, i.e.

$$z = \sum_{ip} \alpha_{ip} w_{ip} , \qquad \alpha_{ip} = w_{ip}^\dagger z . \tag{42}$$

We calculate now

$$A^n z = \sum_{ip} \alpha_{ip} A^n w_{ip} = \sum_{ip} \alpha_{ip} \lambda_i^n w_{ip} = \lambda_1^n \left\{ \sum_p \alpha_{1p} w_{1p} + \sum_{i>1,p} \alpha_{ip} \left(\frac{\lambda_i}{\lambda_1} \right)^n w_{ip} \right\} , \tag{43}$$

$$\|A^n z\| = \sqrt{(A^n z)^\dagger (A^n z)} = \left\{ \sum_{ip} |\alpha_{ip}|^2 \lambda_i^{2n} \right\}^{1/2} = \lambda_1^n \left\{ \sum_p |\alpha_{1p}|^2 + \sum_{i>1,p} |\alpha_{ip}|^2 \left(\frac{\lambda_i}{\lambda_1} \right)^{2n} \right\}^{1/2} , \tag{44}$$

$$v = \lim_{n\to\infty} \frac{A^n z}{\|A^n z\|} = \lim_{n\to\infty} \frac{\sum_p \alpha_{1p} w_{1p} + \sum_{i>1,p} \alpha_{ip} \left(\frac{\lambda_i}{\lambda_1} \right)^n w_{ip}}{\left\{ \sum_p |\alpha_{1p}|^2 + \sum_{i>1,p} |\alpha_{ip}|^2 \left(\frac{\lambda_i}{\lambda_1} \right)^{2n} \right\}^{1/2}} = \frac{\sum_p \alpha_{1p} w_{1p}}{\sqrt{\sum_p |\alpha_{1p}|^2}} . \tag{45}$$

In the last step we have used the fact that $\lambda_i/\lambda_1 < 1$ for $i > 1$ and therefore $\lim_{n\to\infty}(\lambda_i/\lambda_1)^n = 0$. Also notice that the last step makes sense only if $\sum_p |\alpha_{1p}|^2 \neq 0$, which provides a condition on z.

Since v is a linear combination of eigenvalues w_{1p}, it is itself an eigenvector of A with eigenvalue λ_1.

The vector v in eq. (40) can be constructed iteratively. Define

$$v_0 = z , \tag{46}$$

$$v_n = \frac{A v_{n-1}}{\|A v_{n-1}\|} , \quad \text{for } n \geq 1 . \tag{47}$$

Notice that

$$v_{n-1} = \frac{A v_{n-2}}{\|A v_{n-2}\|} , \tag{48}$$

$$A v_{n-1} = \frac{A^2 v_{n-2}}{\|A v_{n-2}\|} , \tag{49}$$

$$\|A v_{n-1}\| = \frac{\|A^2 v_{n-2}\|}{\|A v_{n-2}\|} , \tag{50}$$

$$v_n = \frac{A v_{n-1}}{\|A v_{n-1}\|} = \frac{\frac{A^2 v_{n-2}}{\|A v_{n-2}\|}}{\frac{\|A^2 v_{n-2}\|}{\|A v_{n-2}\|}} = \frac{A^2 v_{n-2}}{\|A^2 v_{n-2}\|} . \tag{51}$$

By iterating this calculation one finds

$$v_n = \frac{A v_{n-1}}{\|A v_{n-1}\|} = \frac{A^2 v_{n-2}}{\|A^2 v_{n-2}\|} = \frac{A^3 v_{n-3}}{\|A^3 v_{n-3}\|} = \cdots = \frac{A^n v_0}{\|A^n v_0\|} = \frac{A^n z}{\|A^n z\|} , \tag{52}$$

which is nothing but the vector inside the limit in eq. (40). This yields

$$v = \lim_{n\to\infty} v_n . \tag{53}$$

Let us denote the largest eigenvalue of A by $\bar{\lambda}$. Since v is a normalized eigenvector of A with eigenvalue $\bar{\lambda}$, we obtain.

$$\bar{\lambda} = \|\lambda v\| = \|A v\| = \lim_{n\to\infty} \|A v_n\| . \tag{54}$$

Therefore, if n is large enough, v_n is a approximation of the eigenvector v, and $\|A v_n\|$ is an approximation of the eigenvalue $\bar{\lambda}$. This observation leads to the following algorithm, which is called *power method*:

1. Choose v randomly.
2. Construct $w = Av$.
3. Calculate $\lambda = \|w\|$.
4. Replace $v \leftarrow w/\lambda$.
5. Repeat from 2 until some stopping criterion is satisfied.
6. Return v as the approximated eigenvector, and λ as the approximated largest eigenvalue.

Exact eigenvalue and eigenvector would be obtained as limits by repeating this algorithm infinitely. The algorithm must be stopped when the approximation is satisfactory. For instance one can stop the algorithm when the eigenvalue equation is satisfied up to some tolerance ϵ, i.e.

$$\|Av - \lambda v\| < \epsilon \ . \tag{55}$$

The tolerance ϵ becomes an input of the algorithm.

One important point to notice is that the power method only needs (in point 2) a function that takes a vector v and returns the vector Av. In particular A does not need to be stored as a matrix anywhere. This point is particular important for sparse matrices, such as the Hamiltonian: saving the whole matrix would be a massive waste of memory, moreover the matrix-vector multiplication would multiply zero times some number most of the time which leads to a loss of efficiency. In the case of sparse matrices with a known structure, Av can be generally constructed more efficiently without storing the matrix A at all. In conclusion, your implementation of the power method, must take a *function* as an input, and not a matrix.

6.2 Conjugate gradient

Given a positive definite square matrix A and a vector b, the conjugate gradient calculates an approximation of $A^{-1}b$. As the power method, the conjugate gradient is an iterative method. A discussion of the conjugate gradient can be found on Wikipedia at `https://en.wikipedia.org/wiki/Conjugate_gradient_method`.

6.3 Lowest eigenvalue and corresponding eigenvector

Let A be a positive definite matrix. If λ_i are the eigenvalues of A and w_i are the corresponding eigenvectors, then

$$Av_i = \lambda_i v_i \quad \Rightarrow \quad A^{-1}v_i = \lambda_i^{-1}A^{-1}(\lambda_i v_i) = \lambda_i^{-1}A^{-1}(Av_i) = \lambda_i^{-1}v_i \ , \tag{56}$$

i.e. v_i are also eigenvectors of A^{-1} and the corresponding eigenvalues are λ_i^{-1}. Since all $\lambda_i > 0$ it follows immediately that λ **is the smallest eigenvalue of** A **if and only if** λ^{-1} **is the largest eigenvalue of** A^{-1}. Moreover **the eigenvector of** A **associated to its smallest eigenvalue coincides with the eigenvector of** A^{-1} **associated to its largest eigenvalue**.

Therefore, the smallest eigenvector of A and its associated eigenvector can be obtained by applying the power method to A^{-1}. The power method requires a function $v \mapsto A^{-1}v$, and this is obtained by applying the conjugate gradient.

By applying this idea to the case $A = \hat{H}_a$, one can write a program to calculate the ground state and ground energy of the considered quantum-mechanical system.