Experiments of Computational Physics - Final essay

Federico De Matteis

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Indice

1 Quantum mechanics on a discete lattice

Solving quantum mechanical problems at the computational level leads us to a representation problem, as the quantum state of a system belongs to an infinite dimensional hilbert space. The computational approach introduce two approximations indeed: the first is called infrared cutoff and consists of imposing an upper limit to the region in which the problem is represented, the second is called ultraviolet cutoff and has to do with the way in which it discretizes that region of space. We will first transpose the study of quantum mechanics problems on a discrete lattice and find the spectra of quantum mechanics hamiltonian, then we will focus on time dependent Schrodinger equation, starting from the kinetic term, the Laplacian operator, and we will discuss some of its usefull charachteristics. We will later discuss the choice of optimal lattice spacing which gives the correct scaling dimension to the terms involved.

2 Laplacian Discretization in 1D

We want to find a discrete representation of the second derivative, in other words we want to construct the Laplacian of a discrete lattice, the kinetic term of the Schrodinger equation. Starting from Taylor's series to the second order we can, in general, rewrite the second derivative bringing it back to a linear form.

$$2f(x) - f(x+a) - f(x-a) \simeq -a^2 \frac{\partial^2}{\partial x^2} f(x)$$

We consider a as the step dx on the discrete lattice. By dividing now by a^2 we obtain a representation of the second derivative with correct scaling dimensions. We can write those information in the form

$$-\frac{\partial^2}{\partial x^2} \to \frac{1}{a^2}\Delta \qquad (\Delta f)_n = 2f(x_n) - f(x_{n+1} - f_{n-1})$$

The Laplacian operator obtained by this procedure is a symmetric operator (i.e., it is a symmetric matrix).

It is important to stress that this version of the discrete laplacian takes in consideration only the first neighbors of the point on which we compute the second derivative. We call the order of this Laplacian p; in the tridiagonal case p=1.

2.1 Translations generator

The operator $-i\frac{\partial}{\partial x}$ is generator of translations. We know the Fourier transform diagonalizes the translations: the Fourier space is the one in which the traslation matrix is diagonal; eigenfunctions for the Fourier space are the plane waves and their eigenvalues the phase factors

$$e^{ik(x-a)} = e^{ikx} \cdot e^{-ika}.$$

If the function whose translation we want to perform is defined on a discrete lattice, the translation occurs by an integer multiple of the lattice step. We ask ourselves what is the finite dimensional matrix that realizes the translation. We think in this regard of an example that is easy to visualize in Matlab; we choose a one-dimensional latex of dimension 12; to do so, we directly define its adjacency matrix with the commands:

$$T = diag(ones(11,1),1) \;\; T(end,1) = 1$$

i.e., a matrix with unitary elements on the upper diagonal and periodic boundary conditions on a ring graph. T translates the elements of a vector to the left;

```
T=diag(ones(11,1),1);
T(end,1)=1;
v=(1:12)';
t=T*v;
disp(t')
%this gives the result:

 t' = 2 3 4 5 6 7 8 9 10 11 12 1
```

If we raise T to the twelfth power we get the identity matrix $T^{12} = I$. This means that the eigenvalues in question e^{-ikb} are (in this case twelfth) roots of order n of the unity and so k is discretized. This is why k must be finite and it cannot be arbitrarily large because $e^{-ikb \cdot n}$ must result in the identity.

To perform a translation of L (length of the ring) must be equal to perform the I operation, which means that $e^{-ikL} = I$, implying $k = \frac{2\pi}{L} \cdot n$ where n is an integer $n = 0, 1, 2, ..., N$

$e^{-ikb} = 1$ and $k = \frac{2\pi}{L}$ is an integer value. The eigenvalues will be displayable, since they are in finite number.

note that: we call the lattice step : $dx = a$.

2.2 Translation matrix and Tridiagonal discrete laplacian

As we know that the translation operator is diagonal on Fourier space we can construct the object

$$T + T'$$

This is the periodic lattice adjacency matrix. If we perform a second operation

$$L = 2 \cdot I(N) - T - T' \quad N = 12$$

we find nothing less than the Laplacian in the tridiagonal form, just written through the second order Taylor series as seen before. When written this way we see that L is diagonal if T is diagonal. L (or Δ) is diagonalized in Fourier space, that corresponds to say that the derivatives are diagonalized by the Fourier transform. There is a clear dichotomy between the adjacency matrix of a periodic graph, on which translations can be performed to the left and right of the considered point, and the second derivative as a function of translation matrices.

L =

2	-1	0	0	0	0	0	0	0	0	0	-1
-1	2	-1	0	0	0	0	0	0	0	0	0
0	-1	2	-1	0	0	0	0	0	0	0	0
0	0	-1	2	-1	0	0	0	0	0	0	0
0	0	0	-1	2	-1	0	0	0	0	0	0
0	0	0	0	-1	2	-1	0	0	0	0	0
0	0	0	0	0	-1	2	-1	0	0	0	0
0	0	0	0	0	0	-1	2	-1	0	0	0
0	0	0	0	0	0	0	-1	2	-1	0	0
0	0	0	0	0	0	0	0	-1	2	-1	0
0	0	0	0	0	0	0	0	0	-1	2	-1
-1	0	0	0	0	0	0	0	0	0	-1	2

2.3 Finite Fourier Transform

The Fourier transform of a complex vector y with n elements in position space is a complex vector Y with n elements in momentum space.

$Y = fy$ where f is a finite-dimensional matrix transformation between the space of positions and its dual; to go from the space of moments to the space of positions we can perform the antitransform f^{-1}.

For the Fourier transform it holds that $F^H F = nI$, where F^H is the conjugate Hermitian matrix of F; we recall that F is a unitary matrix, because it preserves norms; it "moves" between two spaces with basis vectors with unitary norm.

$$F^{-1} = F^H, \quad \sum |Y_j|^2 = \sum |y_j|^2$$

Eigenvalues for an identuty matrix are phase factors, and in the discrete case $\sum_j \omega_j = 0$ i.e. the sum of all n-hex roots of unity makes 0, because they are arranged symmetrically around the point (0,0).

2.4 FFT for periodic boundary conditions

Suppose we are working on a finite space with periodic boundary conditions. Let's remark that the operation we did in discretizing the position space is $x \to x_j = -\frac{N+1}{2}a + ja$ where $j = 1, 2, ..., N$ and $L = Na$.

The momentum takes the values $k_n = \frac{2\pi}{L} n$.

We have to deal with two possible situations: n= $\begin{cases} -\frac{N}{2}, ..., 0, ... \frac{N}{2} - 1 \;\; for \;\; even \;\; N \\ -\frac{N-1}{2}, ..., 0, ... \frac{N-1}{2} \;\; for \;\; odd \;\; N \end{cases}$

We can write explicitly the product

$$k_n \cdot x_j = \frac{2\pi}{L}(-\frac{N+1}{2}a + ja) = -\frac{\pi}{N}(N-1)n + \frac{2\pi}{N}n(j-1)$$

Given a function Y_q we write the representation of its discrete fourier transform as y_j

$$Y_q = \sum_{j=1}^{N} y_j e^{-\frac{2i\pi}{N}}(q-1)(j-1) \quad y_j = \frac{1}{N}\sum_{q=1}^{N} Y_q e^{\frac{2i\pi}{N}(q-1)(j-1)}$$

So the fourier coefficient for a function f, in a more general sense will be

$$f_n = \frac{1}{L}\sum_{j=1}^{N} a f(x_j) e^{-ik_n x_j} = \frac{1}{N} e^{i\pi(1-\frac{1}{N})n} \sum_{j=1}^{N} f_j e^{-\frac{2i\pi}{N}(q-1)(j-1)} = \frac{1}{N} e^{i\pi(1-\frac{1}{N})n} F_q$$

Where we defined

$$p = \frac{N-1}{2} \quad and \;\; so \;\; n = 0, ..., p \;\; q = n+1$$

We obtain the continuum limit of the fourier transform by switching to the integral in the limit of $L \to \infty$

$$f(x) = \sum_{n=\infty}^{\infty} \hat{f}_n e^{ik_n x} = \frac{L}{2\pi} \sum_{n=-\infty}^{\infty} \frac{2\pi}{L} \hat{f}_n e^{ik_n x} \simeq \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \hat{f}_k e^{ikx} \quad and \quad \hat{f_{k_n}} = L\hat{f}_n$$

2.5 FFT for Dirichlet and Newmann boundary conditions

As the fourier transform diagonalizes the laplacian operator on a space with periodic boundary conditions, sine and cosine fourier transform find their application for other spaces.

For a space with Dirichlet boundary conditions we define the sine Fourier transform of a function $x = 1, ..., N$ and $k_n = \frac{\pi}{N+1} n$.

$$f(x) = 2i \sum_{0}^{\infty} \hat{f}_n sink_n x$$

$$\hat{f}^s_n = \sqrt{\frac{2}{L}} \int_0^L dx f(x) sink_n x = i\sqrt{2L}\hat{f}_n$$

For a space with Newmann boundary conditions $x = 0, 1, ..., N-1$ and $k_n = \frac{\pi}{N} n$. We define the cosine Fourier transform

$$f(x) = \hat{f}(0) + 2\sum_{n=1}^{\infty} \hat{f}_n cosk_n x = \sqrt{\frac{1}{L}}\hat{f}^c_0$$

$$where \quad \hat{f}^c_0 = \sqrt{L}\hat{f}_0 = \sqrt{\frac{1}{L}}\int_0^L dx f(x) \quad and \quad \hat{f}^c_n = \sqrt{2L}\hat{f}_n = \sqrt{\frac{2}{L}}\int_0^L dx f(x) cosk_n x$$

2.6 First derivative as non local operator

We try to obtain the first derivative operator by the same method used for the Laplacian. One way to obtain the discrete derivative might be to write the operator

$$D_+ = \frac{1}{a}(T - I) = \frac{1}{a}(f(x+a) - f(x))$$

and its complex conjugate

$$D^\dagger_+ = D_- = I - T^\dagger = \frac{1}{a}(f(x) - f(x-a))$$

These operators take the difference between one point and the next or previous point; the problem is that none of these operators are symmetric. We note that these operators give us a second operational way to write the Laplacian, which is a real and symmetric matrix

$$D+ \cdot D- = -\Delta$$

We could actually perform a semi-sum of D_+ and D_- to get a symmetric operator, which would correspond to the operation

$$\frac{1}{2}(f(x+a) - f(x-a))$$

However, this operator is blind to functions that change sign between lattice points.

"There are no local rapresentation for the first derivative, the momentum is a non local operator, and either there are no local representations for $\hat{k}$ as a diagonal matrix with bands".

We already have a representation of the impulse: it is just $\hat{k}$ already diagonal in fourier space, it is the wave number; we can then obtain the discrete derivative using the fast fourier transform.

2.7 Quantizing k

We can resume the results about the Fourier transform. Depending on the boundary conditions we need to represent the lattice, the momentum $\hat{k}$ is quantized as follows

- PBC: $k = \frac{2\pi q}{N}$ where $q = -\frac{N}{2}, .., 0, .., \frac{N}{2} - 1$ for N even,
  $q = -\frac{N-1}{2}, .., 0, .., \frac{N-1}{2}$ for N odd
  the eigenvectors are $u_{kn} = \frac{1}{\sqrt{N}} e^{ikn}$.
  In this case the Laplacian is diagonalized by the Fourier transform.

- DBC: $k = \frac{\pi q}{N+1}$ where $q = 1, 2, 3, .., N$ and the eigenvectors are $u_{k_n} = \sqrt{\frac{2}{N+1}} sin(kn)$.
  The laplacian is diagonalized by the sine Fourier transform.

- NBC: $k = \frac{\pi q}{N}$ where $q = 0, 1, 2, 3, .., N-1$ and the eigenvectors are $u_{k_n} = \sqrt{\frac{2}{N}} cos(k(n - \frac{1}{2}))$.
  The laplacian is diagonalized by the cosine fourier transform.

The eigenvalues of the Laplacian with periodic boundary conditions (PBC) are easily obtained from $\Delta u_k = \hat{k}^2 u_k$ with

$$\hat{k} = 2sin(\frac{k}{2})$$

if the lattice spacing is $a = 1$. For Newmann and Dirichlet boundary conditions prostaferesys formulas lead us to eigenvalues.

2.8 Multidiagonal discrete Laplacian

If we generalize the concept of the previous definition for the laplacian of a function to the order p we will obtain the multidiagonal form of the laplacian; in this definition we extend the number of first neighbors points taken in consideration in the expansion in Taylor series of the second derivative from the point x_n.

$$2\alpha_0 f(x) + \alpha_1[f(x+a) + f(x-a)] + \alpha_2[f(x+2a) + f(x-2a)] + ... =$$

$$= \sum_{j=0}^{p} \alpha_j[f(x+ja) + f(x-ja)] \simeq -a^2[\frac{\partial^2}{\partial x^2} f(x) + O(a^{2p})]$$

In the limit of p=1 we return to the definition of the tridiagonal form Laplacian. In a sparse form we can represent it as follows

$$M = \begin{pmatrix} 2 & 2 & 2 & \dots & 2 \\ 0 & 1 & 2^2 & \dots & p^2 \\ 0 & 1 & 2^4 & \dots & p^4 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 1 & 2^{2p} & \dots & p^{2p} \end{pmatrix} \cdot \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_p \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

This system can be solved with a backslash operator as a system of linear equations , considering the α vector as incognita. Eigenvalues equation in the most general sense takes the form

$$\lambda(\Delta^{(p)} = \hat{k}^2) = 2\sum_{s=0}^{p} c_s^{(p)} cos(sk)$$

Eigenvectors takes the form just discussed for the tridiagonal discrete Laplacian in the three boundary conditions hypothesis.

2.9 Infinite order discrete Laplacian

It is possible to extend the definition of the laplacian of order p to $p = \infty$; the expressions for eigenvectors are the same as in the cases of tridiagonal and multidiagonal Laplacians. Eigenvalues take the form

$$\lambda(\Delta^{(p)}) = \lim_{p\to\infty} 2\sum_{s=0}^{p} c_s^{(p)} cos(sk) = \hat{k}^2$$

The first coefficient takes the form $c_0^{\infty} = \frac{\pi^2}{6}$ and the last one $c_s^{\infty} = 2\frac{(-1)^s}{s^2}$ where $s = 1, 2, ...$, as a result of a very well known cosine series.

As we know the eigenvalues we also know the diagonal matrix expression for $\Delta_{diag}^{(\infty)}$ in the basis of its eigenvectors

$$\Delta^{(\infty)} = F\Delta_{diag}^{(\infty)}F^{-1}$$

The matrix that diagonalizes it, is the Fourier transform in one of the three forms.

We will use the infinite order laplacian later to enhance the accuracy of this method compared to the tridiagonal method for the harmonic oscillator spectrum.

3 The path to Schrodinger equation

We can introduce the missing part of the Schrodinger equation, the potential $V(x)$.

$$H = -\frac{1}{2}\Delta + V(x)$$

In the following we will consider $\hbar = m = 1$.

The potential energy matrix is diagonal with respect to the basis position , and so the fourier space is not the space in which the entire hamiltonian is diagonal, as the commutator $[V, \Delta] \neq 0$. Δ is diagonal on the fourier basis of the hermite polynomials; however, it is not enough to know Laplacian's eigenvalues to solve the problem from now on, except for the case of the harmonic oscillator $V(x) = \frac{1}{2}\omega^2 x^2$.

As we remember from classical mechanics the hamiltonian of the harmonic oscillator is invariant under fourier transform and so the Poisson parenthesis are conserved under that transformation; that means that the fourier space is still the space in which the hamiltonian is diagonal. The harmonic oscillator will be used next as an example of solving the eigenvalues equation for the hamiltonian.

3.1 Harmonic oscillator

Let's take in consideration the hamiltonian of the harmonic oscillator

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2$$

```
function harmonic_quant_waves
j=1;
N=j*1000;
%optimal lattice spacing
maxV = 0.5*(N/2)^2;      % not exact but very close
maxT = pi^2/2;           % not exact (for DBC and NBC) but very close
a = (maxT/maxV)^(1/4);   % "optimal" lattice spacing: see notes on this topic
```

```
% the grid
x = -(N-1)/2:(N-1)/2;
x = a*x';
%x=linspace(-10,10,j*1000);
%a=(x(2)-x(1));

T=diag(ones(N-1,1),1);
T(N,1) = 1;                    %imposing periodic boundary conditions (PBC)

L=(2*eye(N)-T-T')/a^2;
H=0.5*L+0.5*diag(x.^2);
[u,e]=eig(H);
e=diag(e);
```

Here we used the algorithm qharmoscpsi.m which provides eigenfunctions of the quantum harmonic oscillator $H = p^2/2 + q^2/2$ (so in this evaluation $\omega = 1$), evaluated over the zeros of H_n, the Hermite polynomial of order n. We confront those eigenfunctions in their functional representation with the numerical values found using the eig algorithm on the hamiltonian, in order to check accuracy. We did it using the script hamiltonian 1D in order to confront the multidiagon and tridiagonal methods for gaining the spectrum of H.

Running the code above we obtain the two spectra of the harmonic oscillator made of 1000 eigenvalues; we note that the effect of finite dimensionality is to miscalculate eigenvalues correnspondent to eigenfunctions that are not well contained in the finite volume (i.e. infrared cut-off effects).

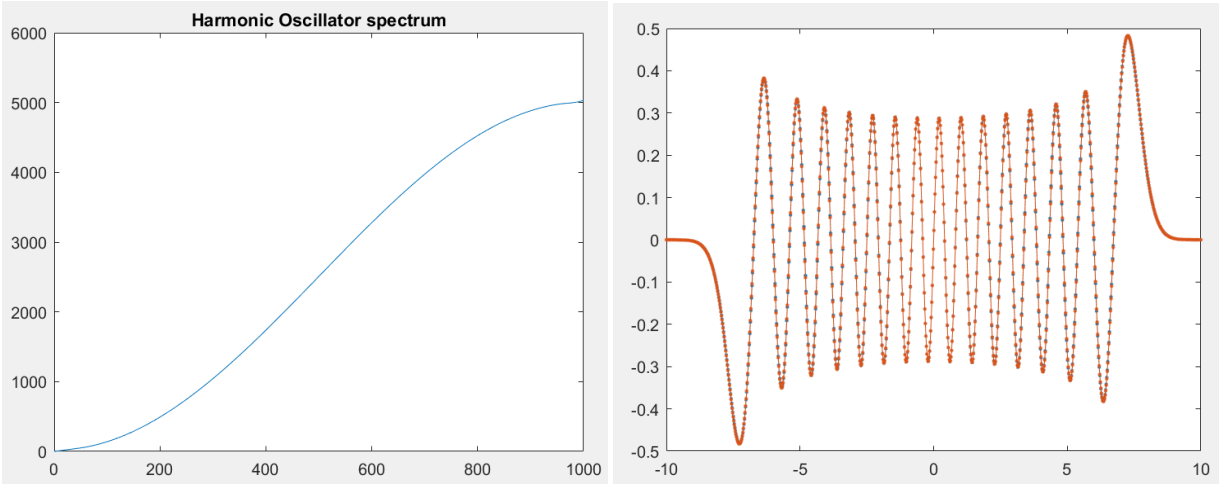


Figura 1: Harmonic oscillator spectrum, obtained without using the choice of optimal lattice spacing, as done in the code above; we bring this image as a comparison with the oscillator spectrum in the next image. In the second image we can see the thirtieth eigenfunction for the harmonic oscillator

In the second plot we see the thirtieth eigenfunction of the harmonic oscillator obtained with the two methods, almost totally superimposed. We note that it is well sampled and practically null at the edges of the volume for both methods; if we tried to plot higher order eigenfunctions we would notice an increasing departure from the correct functional form that is calculated with qharmoscpsi.

An instructive example is that of eigenfunctions with a very high value of n (i.e. n=500). In this case we would notice a bad behaviour due to an infrared cutoff, because of the function bangs against the edges of the volume, but also a bad behaviour due to an UV cutoff,in fact the function oscillates too fast within a translation smaller than the lattice spacing. It is a problem that can be solved by thickening the lattice and looking for the continuum limit. We underline a behaviour for the harmonic oscillator: IR and UV effects occur at the same time.

This does not happen for spectrum of the harmonic oscillator in the Occupation Number representation, for which instead eigenfunctions are "exact in number approximation" from the first to the last, showing a good behaviour in terms of IR cutoff in the space of the position, which is reflected by good sampling in the UV sense in the fourier space.

3.2 Infinite order Laplacian and the spectrum of harmonic oscillator

We use the fourier transform to write the Hamiltonian in its tridiagonal form; we also define the Laplacian in its infinite form using the "inverse fourier transform method". The infinite order form is the most accurate as a limit to the continuum representation; starting from the code used previously we can write

```
%coefficients for the infinite order laplacian
n = floor(N/2);
nn = floor((N-1)/2);
k = (2*pi/N)*(-n:nn)';

L = ifft(diag(fftshift(k.^2))*fft(eye(N)));    % Laplacian in Fourier space

L = real(L+L')/2;                              %this makes L exactly symmetric
V= 0.5*diag(x.^2);
H = L/2/a^2 + V;

E = eig(H);
Etri = eig(Htri);
```

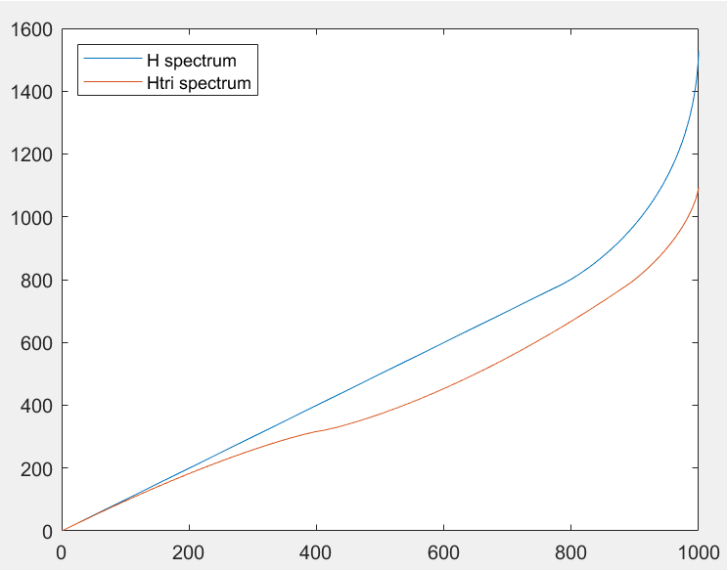
This is a second method to represent the laplacian operator; it transforms the diagonal matrix whose eigenvectors are the plane waves with the fourier transform, and after multiplying for the coefficients k^2, it brings the object back to the position basis by applying the inverse fourier transform.

$$\Delta^{(p)} = F^{-1}\Delta_{diag}F \quad F^{-1}=F^{\dagger}$$

$$F^{-1}\Delta^{(p)}u_k = F^{-1}k^2u_k$$

This is exactly like resolving an eigenvalues equation for Δ. In this particular case we use the classic finite fourier and its inverse, by this approach the inverse fourier will give us a laplacian operator defined on a space with Periodic Boundary Conditions (PBC). Is is important to remember that for other boundary conditions like DBC's and NBC's the laplacian is diagonalized by the cosine and sine Fourier transforms.

With this method we obtain a full matrix (infinte p order) laplacian and we solve the eigenvalues equation for H with the usual method.



Spectra of H tridiaonal versus H infinite order

Figura 2: Tridiagonal spectrum gives non-stable eigenvalues for more eigenvectors, we expect the spectrum of the harmonic oscillator to have a linear behaviour (eigenvalues grows linearly)

The code written above gives the eigenvalues for the Hamiltonian in tridiagonal and multidiagonal forms; the plot in figure 2 plot was made of the two spectra for both hamiltonians. On one hand the spectrum of the tridiagonal hamiltonian is affected by the bad quantization of the Laplacian, on the other the multidiagonal form provides a more stable spectrum that remains linear for eigenfunctions with higher principal quantum numbers (which are the eigenfunctions that typically oscillate faster and have non-negligible values at the edges of the volume).

We enhance that through the use of Fourier transform involves a relevant computational gain; the computational cost of a matrix multiplication is of order N^3, while diagonalization in Fourier basis permits to perform the same operation in the Fourier space, with a cost of $N\log_2(N)$.

4 Time dependent Schrodinger equation

In this section we focus on the time evolution of a quantum state and the Time Evolution operator. The time evolution of a state $\Psi(t)$ can be obtained by the action of the Time Evolution operator written in the form

$$U(t_0 + \epsilon, t_0) = I - i\epsilon H dt$$

Applying the compository rules between different times $t_0 < t_1 < t_2$ we get to

$$U(t + dt, t_0) - U(t, t_0) = -iHdtU(t, t_0)$$

By expanding the left side as a Taylor series we find

$$i\frac{\partial}{\partial t}U(t, t_0) = HU(t, t_0)$$

This is the Schrodinger equation for the time evolution operator; since the initial state $|\Psi(x, t_0) >$ is time t independent we can write the Schrodinger equation as follows

$$i\frac{\partial}{\partial t}|\Psi(x, t_0), t >= H(t, t_0)|\Psi(x, t_0), t >$$

We are interested in studying cases of non time dependent hamiltonians for which the solution to the Schrodinger equation written above is

$$U(t, t_0) = e^{-iH(t-t_0)}$$

4.1 Operator splitting technique

Let's take in consideration the hamiltonian written as

$$H = H_0 + V \;\; where \;\; H_0 = -\frac{1}{2}\frac{\partial^2}{\partial x^2}$$

We can perform the time evolution operator on a state, reducing computational complexity and execution time, approximating it with a new operator. We consider the time evolution $U(t) = e^{-}iHt$, and a finite timestep τ. The total time taken in consideration will be $\tau n = t$

$$U(t) = [e^{-}iH\tau]^n$$

Now we actually do the approximation

$$U(\tau) \simeq \hat{U(\tau)}$$

where we are leaving by the term $\sigma(\tau^3)$ in the right side of the approximation and

$$\hat{U(\tau)} = e^{-iV\frac{\tau}{2}}e^{-iH\tau}e^{-iV\frac{\tau}{2}}$$

The equivalence $U(\tau) = U(\tau) \hat{+} o(\tau^3)$ is true for sufficiently small τ. In the position space the operator $e^{-iV\frac{\tau}{2}}$ is diagonal because diagonal is the matrix V. The term $e^{-iH_0\tau}$ is diagonal on the fourier basis, for this reason we can write

$$e^{iH_0\tau} = F^{-1}e^{-i\frac{k^2}{2}\tau}F$$

This way we bring the term $e^{-iV\frac{\tau}{2}}|\Psi(x, t_0)$ in the Fourier space and perform a product with the diagonal kinetic term; then the inverse fourier transform takes the object $e^{i\frac{k^2}{2}\tau}e^{-iV\frac{\tau}{2}}|\Psi(x, t_0)$ back to the position space, in which the last product with $e^{-iV\frac{\tau}{2}}$ is performed. Using the operator splitting we are able to reduce the time cost of calculating the time evolution: we obtain the Laplacian through the fast fourier transform and we calculate a product between a vector and a diagonal matrix (in Fourier space).

4.2 Quantum Tunneling

We can imagine a wave packet with an initial momentum k_0; Its classical energy is obtained by averaging the energy of its components. Let's imagine the wave packet propagates in the direction of a potential barrier; from a classical point of view there will be a fraction of wave packet that crosses the barrier. Those are the single components of the state that has higher energy than the barrier themselves. In the classical framework the wave packet is interpreted as a statistical distribution.

However, from a quantum mechanics point of view the fraction of the packet crossing the potential barrier is expected to be greater than can it be explained by a classical theory; this phenomenon is due to the Trasmission coefficient of the barrier and it is called quantum tunneling.

We recall that due to the quantum nature of the wave packet the reflection phenomenon is still possible, even if the energy of the component of a state is grater than the barrier. We find the evidence of quantum tunneling in the livescript timeevolution.xlm for a state subjected to a double well potential barrier.

Number Operator and the potential family $V \approx q^{\alpha}$

In this section we want to explore the use of the number operator and study its effect on the calculation of the Hamiltonian spectrum, starting with the quartic oscillator to later adress the harmonic oscillator problem.

Let's start with the creation operator $a^{\dagger}$ and its conjugate complex, the destruction operator a: we can write a representation for the position $\hat{q}$ and the momentum $\hat{p}$ according to $a, a^{\dagger}$:

$$q = \frac{1}{\sqrt{2}}(a + a^{\dagger}) \quad \text{and} \quad p = -\frac{i}{\sqrt{2}}(a - a^{\dagger})$$

We remember that $a|n\rangle = \sqrt{n}\,|n-1\rangle$ and $a^{\dagger}|n\rangle = \sqrt{n+1}\,|n+1\rangle$

and that the solution to the eigenvalues for the Hamiltonian of the harmonic oscillator is

$$H = \frac{p^2}{2} + \frac{q^2}{2} \quad \text{è} \quad H|n\rangle = \left(\mathrm{a}\mathrm{a}^{\dagger} + \frac{1}{2}\right)|n\rangle$$

Eigenvectors $|n\rangle$ have as functional form : the hermite polynomials $\Psi_n(x)$ with $n = 1, \ldots, N$.

We also recall that the application of the position operator on an eigenstate of the harmonic oscillator is given by the recurrence rule: $x\,\Psi_n(x) = \sqrt{\frac{n}{2}}\Psi_{n-1}(x) + \sqrt{\frac{n+1}{2}}\,\Psi_{n+1}(x)$

So if we use the position operator q on an eigenstate of the position base $|x\rangle_N$ we have

$$q|x\rangle_N = x|x\rangle_N - \frac{1}{2}\Psi_{N+1}(x)\sqrt{N+1}\,|N\rangle + \frac{1}{2}\Psi_N(x)\sqrt{N+1}\,|N+1\rangle$$

To transpose this problem onto a discrete lattice, we need to truncate the occupancy number space N, representing the number operator on a finite base, numbered by $n = 0, 1, 2, \ldots, N$. We are no longer able to us $|\,N+1\,\rangle$, because it is not available, therefore the representation of the action of on a state $|x\rangle_N$ reduces to

$$q|x\rangle_N = x|x\rangle_N - \frac{1}{2}\Psi_{N+1}(x)\sqrt{N+1}\,|N\rangle$$

If we choose to reset the last term to zero: $\Psi_{N+1}\left(x_j^{(N+1)}\right) = 0$

we obtain an eigenvalues equation for q for which eigenvalues are just the positions $\left(x_j^{(N+1)}\right)$.

$$q|x_j^{(N+1)}\rangle = x_j^{(N+1)}|x_j^{(N+1)}\rangle \quad with \quad j = 0, 1, ..., N$$

We can assert that the spectrum of the operator q in the truncated space of the occupation number is given by the zeros of the Hermite polynomial $\Psi_{N+1}(x)$, which are nothing more than the positions x_j of the discrete graph obtained from the diagonalization of $\hat{q}$.

Truncating the occupation number to finite N is equivalent to not use the series of hermite polynomials of higher order to N: $N+1, \ldots, \infty$; in an ideal world the occupation number would not be truncated and the eigenvalues of q would be all the x's on the real axis.

The volume (L) in which we represent the problem is automatically determined by $L = \mathrm{Na}$.

```
%we choose to cut the representation to an occupation number N=2e3
N=1e3;
%defining a and a' on the truncate space
a = diag(sqrt(1:N-1),1);
%defining q on the truncate space
q = (a+a')/sqrt(2);
%defining N on the truncate space
H0 = diag((0:N-1)+1/2);
```

$H_0 = \mathrm{diag}\left(N + \frac{1}{2}\right)$ is the Hamiltonian of the harmonic oscillator in base of the number operator; here the Hamiltonian is diagonal and its as eigenvalues are those just seen; Let's start by representing the Hamiltonian of the quartic oscillator $H_{\mathrm{quartic}} = \frac{p^2}{2} + \frac{q^4}{24}$. We want to get this Hamiltonian from the number operator e and to do so we write $H_{\mathrm{quartic}} = H_0 - \frac{q^2}{2} + \frac{q^4}{24}$; We need to use the matrix expression of the operator and derive its eigenvalues

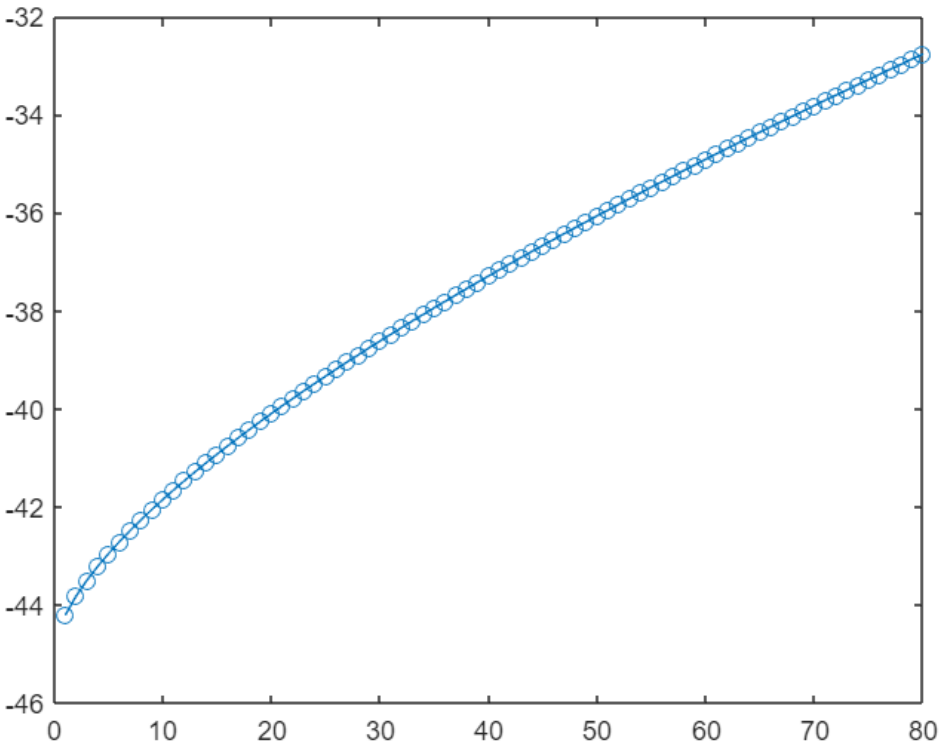
```
x = eig(q);
```

Now we are able to represent the quartic Hamiltonian on the basis of the number operator; the last consideration to do before solving the spectrum of the quartic oscillator is the one concerning the scale size.

We estimate the dependence of the operators kinetic energy T and potential V from the lattice step, which in turn is uniquely determined from the truncated occupation number N and to do so we take into account the approach already used; the potential V is written as $V \approx q^4$; it is clear that the trend of the operator q is directly proportional to the lattice spacing a in the position space x, i.e. in the "direct" grid $V \approx q^4 \approx a^4$ (the potential written now in the base of the number operator works as long as the lattice spacing of the direct lattice is equal to 1, this is not our case; the lattice spacing $a$is determined by the maximum number of occupancy).

The kinetic energy this has a dependence of the type $T = \frac{p^2}{2} = \frac{k^2}{2} = \frac{1}{2}\left(\frac{2\pi}{N \cdot a} n\right)^2 \Big|_{n=\frac{N}{2}} = \frac{\pi^2}{a^2}$

```
plot(x(1:80),'o-')
```



Here we can see a plot of the grid for the first 80 positions; we note that the direct lattice has a lattice spacing that decreases as we move away from the origin because the zeros of the hermite polynomials are not equally distributed in the lattice. The area near the origin 0 and the extreme N is sampled less densely.

There is a theorem wich can help us to understand how zeros of Hemrite polinomials distibute over the real axes for increasing occupation numbers.

Theorem: Let x1 < ... < xn be the zeros of H_n, and let $\mathrm{y1} <\ldots< \mathrm{yn}+1$ be the zeros of H_{n+1} then $a < \mathrm{y1} < \mathrm{x1} < \mathrm{y2} < \mathrm{x2} <\ldots \mathrm{yn} < \mathrm{xn} < \mathrm{yn}+1 < b$, that is, an "interlacing" property between the zeros of Hermite polynomials holds.

We define now for correctness of notation the inverse of the lattice spacing, with which we correct the operators $T,\ V$; the correction to be made is to multiply the operators by the scale magnitude $s = f(a)\ \mathrm{where}\ a\ \mathrm{is\ he\ lattice\ spacing}$, to obtain a representation of the operator scaled with the discrete latex.

The potential reaches the right scale size when multiplied by its scale factor: $V = \frac{1}{24} q^4 \ \rightarrow V = \frac{1}{24}\left(\frac{q}{w}\right)^4$

The same is true for the kinetic energy, for which we get $T = \frac{1}{2} L \rightarrow T = \frac{1}{2} L \frac{1}{a^2} = \frac{1}{2}\mathrm{Lw}^2$

Now we wonder about the latex spacing a (or the "occupation volume" w) for which we have the best representation of the problem from a numerical point of view. We want to make sure that the condition of conservation of energy is satisfied, so we impose that the maximum kinetic energy and the maximum potential

energy are equal (it is equivalent to place equal the energies in the points where T cancels, maximum of V, and where V cancels, maximum of T).

The condition must be imposed by considering the correct scale size

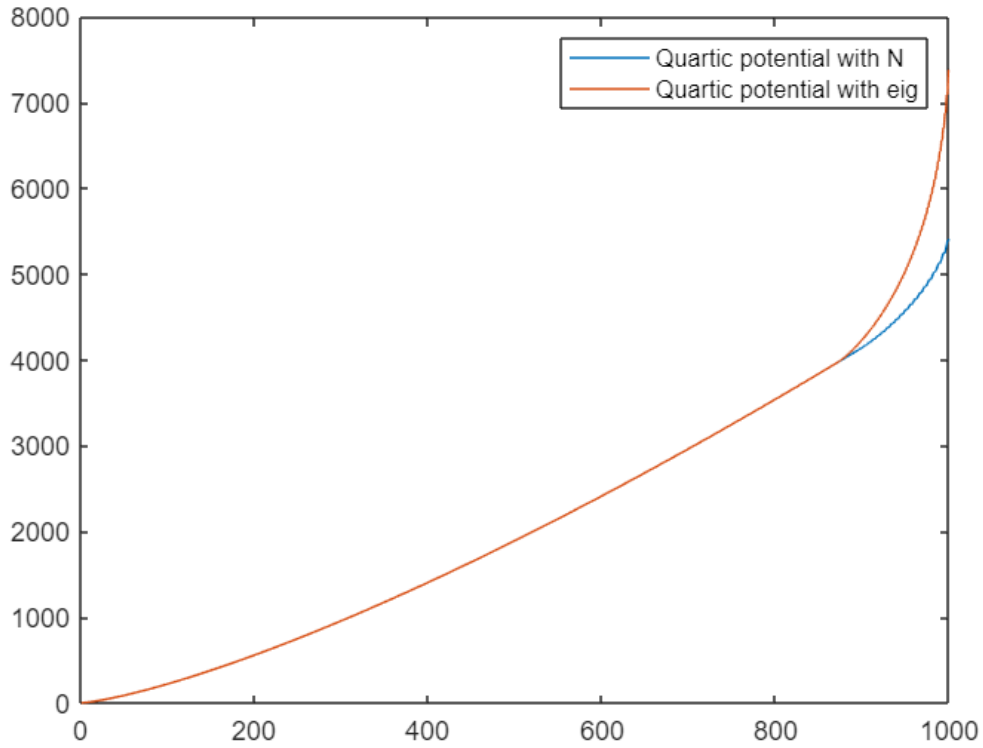
$$T_{\max} w^2 = \frac{1}{2}\max(w \cdot p)^2 = \frac{1}{24}\max\left(\frac{x}{w}\right)^4 = \frac{1}{w^4} V_{\max}$$

and by knowing $\max(p) \simeq \max(x)$ (is true unless a factor π), we obtain $w = \left(\frac{V_{\max}}{T_{\max}}\right)^{\frac{1}{6}} = \left(\frac{\max(x)^2}{12}\right)^{\frac{1}{6}}$

```
inverse_a = (max(x)^2/12)^(1/6); %inva = w = iverse of optimal lattice spacing
```

We finally write the Hamiltonian in which we insert the correct scaling dimensions and find its eigenvalues using the eig algorithm.

```
H_quartic = inverse_a^2*(H0-q^2/2)+(q/inverse_a)^4/24;
e = eig(H_quartic);
%[V,D] = eig(H_quartic);
figure
plot(e)
hold on
eH = Vquartic_eig(N);
plot(eH(:,1))
legend('Quartic potential with N ','Quartic potential with eig')
```



We note that the spectra calculated with the two methods are exactly superimposed for more than 80% of the eigenfunctions;

It is clear that using this procedure to obtain the spectrum of the quartic oscillator is more performant than the diagonalization of a full H matrix, obtained for example using the order form of the Laplacian. This is because, despite eig is used twice the matrices to be diagonalized are: a tridiagonal matrix with the main diagonal consisting only of zeros, and $H_0 - \frac{q^2}{2} + \frac{q^4}{24}$ a matrix written as the sum of a diagonal matrix, H_0, and q^2 e q^4(both diagonalizable matrices); this ensures a lower computational cost than that associated with diagonalizing a generic square matrix.

Last but not least we have to adress the inherent accuracy of this method. The spectrum of the operator H_0 is an exact spectrum by definition; the approximation we are making concerns the truncation of the occupation number and nothing else. The operators involved, in particular T, by construction do not depend on the number of points considered in the lattice. The hermite polynomials computed with qharmoscpsi are exact in precision number.

We repeat the exercise for the harmonic oscillator, but first realize that we can extend the problem to an entire family of potentials of the type $V \approx \text{cost} \cdot q^{\alpha}$, in the most general case then $a = \frac{1}{w} = \left(\frac{T_{\max}}{V_{\max}}\right)^{\frac{1}{\alpha+2}}$; we can evaluate (with qharmoscpsi for example) the exact polynomials and check the accuracy of the representation; in the latter the Hamiltonian H_0 is diagonal and the only diagonalization needed by eig is that of the operator q.

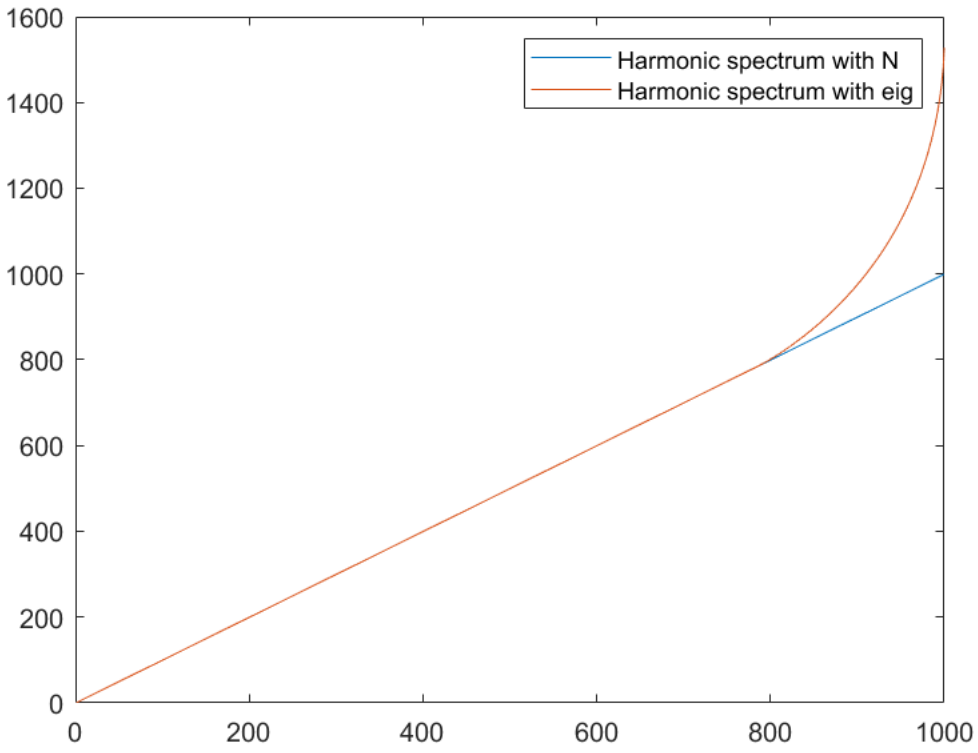
Before turning to the harmonic oscillator we plot the eigenfunctions of the Hamiltonian problem Number of the harmonic oscillator on the grid of positions obtained as zeros of the N+1 hermite polynomial.

Harmonic oscillator within the base of the occupation number N.

We use the eig algorithm to obtain eigenvalues and eigenvectors of the harmonic oscillator Hamiltonian $H = \frac{p^2}{2} + \frac{q^2}{2}$.

```
%defining grid by using Number operators eig equation
[Psi,E] = eig(H0);
%We have the eigenvalues and eigenvectors of the Harmonic Oscillator on the
%basis of the occupation number.
E=diag(E);
figure
plot(E)
hold on
%now we plot the spectra of the harmoni oscilator using Hamiltonian1D, the
%classic PBC Fourier transform method
maxT=(pi^2/2);
%maxT,maxV
V = @(x)x.^2/2;
maxV=V(N/2);
%best lattice spacing for conserving energy
optimaldx=(maxT/maxV)^(1/4);
[H,z,Htri] = hamiltonian1D(N,optimaldx,V,'PBC');
```

```
F=eig(H);
plot(F)
legend('Harmonic spectrum with N','Harmonic spectrum with eig')
```



Spectra with the two methods allow us to estimate how reliable are the eigenstates obtained by diagonalizing H as a multidiagonal matrix of order p-∞ and comparing their accuracy with the exact ones of the number representation. Again, the spectrum obtained with hamiltonian1D is perfectly superimposed on that obtained with the number representation up to very large values of the occupation number.

Time evolution of the Schrodinger equation

Operator splitting and Quantum tunneling

Localized potential & localized state

If there is something that lends itself to solve numerically the time dependent Schrodinger equation this is operator splitting technique.

Let's imagine an Hamiltonian given only by the kinetic term, that is the one of the free particle

$$\widehat{T} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} = \frac{1}{2}\Delta$$

We already know how to diagonalize this finite operator, we can use the finite fourier transform in one of its three acceptions, but we need to discuss the boundary condition of the problem, in order to choose the right one. To do so we have to give a proper example.

We will discuss the time evolution of a localized state which collides against a double well potential barrier.

We define a dimension N for the space grid and a lattice spacing a.

```
N = 2.24e3;
```

Optimal lattice spacing

We impose the conservation of energy condition to find the optimal lattice spacing given the Double Well potential. We write the conservation equation

$T_{\max} = V_{\max}$ where $V = \frac{(x^2 - \text{shift}^2)^2}{24}$ and $T = \frac{1}{2}\frac{k_{\max}^2}{a^2}$; if we substitute the expressions for $k_{\max}$ and $x_{\max}$

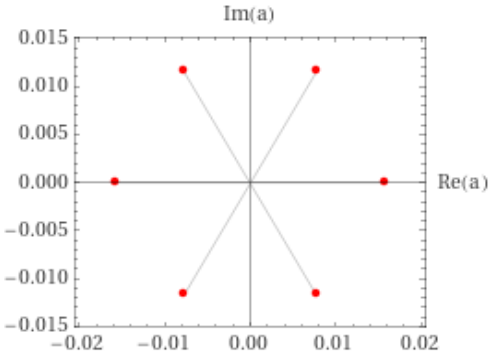
$$k = \frac{\pi}{N+1}n \quad q = -\frac{N-1}{2}, ..., \frac{N-1}{2} \quad and \quad x_{max} = q_{max} = \frac{N-1}{2}$$

the conservation equation becomes the 6th grade equation in a

$$(N)^4\frac{1}{24}a^6 - 2\cdot \text{shift}^2 \cdot N^2\frac{1}{24}a^4 + \frac{\text{shift}^4}{24}a^2 - \pi^2\left(\frac{N}{N+1}\right)^2 = 0$$

where $\text{shift} = \frac{\text{length}(x)}{200}$

and if we solve it for a we will find the six roots shown in the $\text{Wolfram}^{\text{TM}}$ plot



the two real roots are $a = \pm 0.015779$; we will choose the positive root as optimal lattice spacing.

```
a=0.0150984;
%H=hamiltonian1D(N,a,V,'DBC')
x = -(N-1)/2:(N-1)/2;
x = a*x';
shift = length(x)/200; %make the shift of the potential dependent
                       %from the size of the lattice
V= @(x) (x.^2-shift^2).^2/24;
%optimal lattice spacing conserving energy
plot(x,V(x),'.-');
title('Double Well potential')
```

With this approach we obtain a lattice spacing which depends on the shift of the double well. Since the number of points are fixed we have to find the best shift factor for this particular choice of the lattice spacing; Such a shift will allow us to obtain a pronounced double bell potential, like in figure 2 (we choose that a right shift value might be $\approx \frac{\text{length}(x)}{200}$).

Localized state with initial momentum $\widehat{k_0}$

```
k_0 = 10;     % Initial Momentum of a localized state
             % we need to assing an initial momentum to the state by
             % multiplying for the phase exp(i*k_0*x)
            %it fixes a velocity for the wave package (k=2pi/w)

sigma = 0.1;   % initial Gaussian width
psi0 = exp(1i*k_0*x).*exp(-(x+15.25).^2/sigma^2/2); %localized state with momentum
psi0 = psi0/norm(psi0);
psi = psi0;

s=1e4;
hold on
%plot(x,s*abs(psi).^2,'.-')
```

We will use the scale factor s to plot the state ; the scale of the problem is actually fixed by the size of the double well as we have just seen from the optimal lattice spacing equation.

The time evolution of this experiment leads to the collision of the state (which is moving to the right due to its positive k_0) on the barrier and due to the reflection coefficient of the barrier we know that "part" of this wave function is rejected to the left. Therefore the lattice representing the space must not have classic periodic boundary conditions. Actually in the case of PBC the parts of the wavefunction reaching the edges of the finite volume would interfere with each other or at least propagate in the rest of the volume. As we need a space with boundary conditions that zero out the wavefunctions at the edges, we choose the Dirichlet boundary conditions, yet discussed in the Finite Fourier tranform section;

We can define $k_n = \frac{\pi}{N+1} n \quad n = 1 \dots N$ and the kinetc enegy written in term of the momentum $\frac{1}{2a^2} k^2 = T$

```
k = (pi/(N+1))*(1:N)';  % momentum
kinE = (k/a).^2/2;  %Kinetic energy

%single time step size
tau = 0.001;
%time step number   % total time of the simulation is t=10s
nt = 1e3;
```

Operator splitting

We write the approximation for the application of Time Evolution operator as

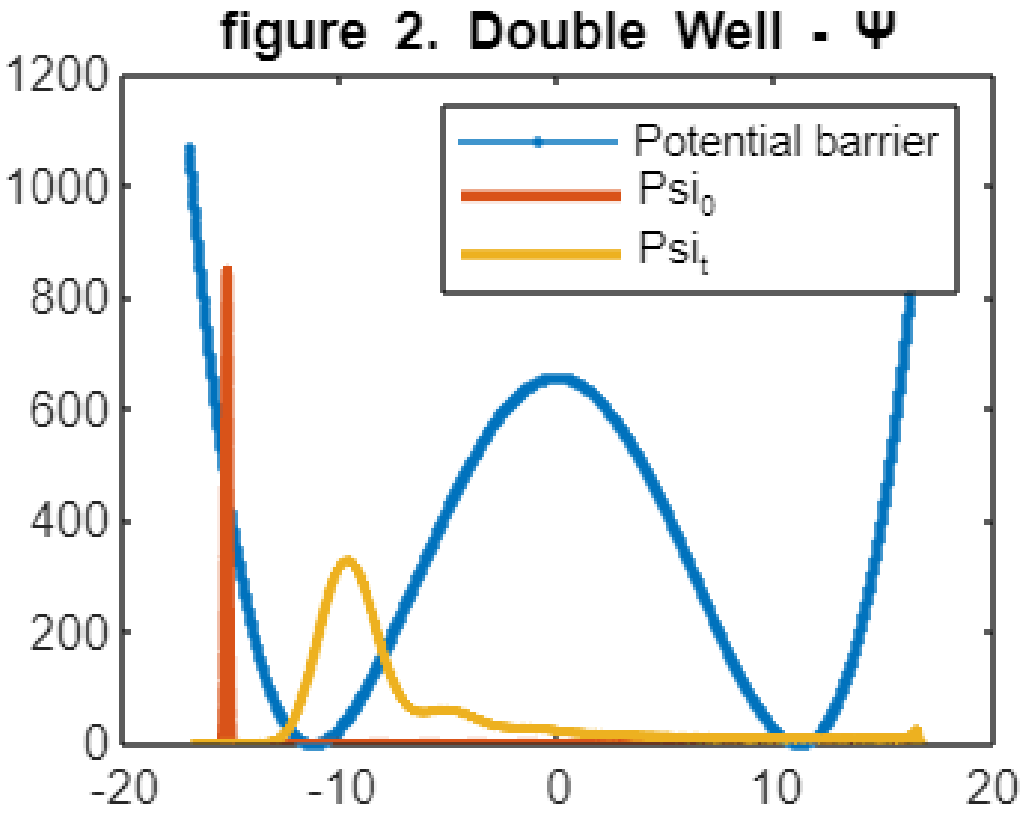
$$\hat{U}\,\Psi = e^{-\mathrm{i}V\frac{\tau}{2}} F^{-1}\left(e^{-i\frac{k^2}{2}} F\left(e^{-\mathrm{i}V\frac{\tau}{2}} \Psi \right) \right)$$

```
if exist('hf','var') && isgraphics(hf)
    hf.YData = s*abs(psi).^2;        %plot dello stato sul grafico
else
    hf = plot(x,s*abs(psi).^2,'linewidth',2);
end
ht = title(sprintf('t = %-5.2f',0));

tic;
for j=1:nt
    psi = exp(-1i*V(x)*tau/2).*psi;
    psi = sinft(exp(-1i*kinE*tau).*sinft(psi));
    psi = exp(-1i*V(x)*tau/2).*psi;
    %if mod(j,5) == 0
    %    hf.YData = s*abs(psi).^2;
    %    ht.String = sprintf('t = %-5.2f',j*tau);
    %    drawnow;
    %end
end
toc;
```

```
Elapsed time is 1.022612 seconds.
```

```
hold on
plot(x,s*10*abs(psi).^2, 'linewidth',2)   %we multiplied s*10 in order to have
                                          %a good visual representation of the final state.
legend('Potential barrier','Psi_0','Psi_t')
title('figure 2. Double Well - \Psi')
```



Classical Energy & Tunnel effect

The state used in the simulation has a starting classic energy at 50.0525; the wave packet has its initial position in a region of space in which the potential is decreasing, toward its first knot ($x \approx 11$), so the state can pass through the barrier reaching the central region. Once there the state crash against a potential barrier which has an higher energy than the initial state. The state must come back, descending again the potential gradient towards the first minimum. From a classical point of view, a wave packet with fixed average energy has components with higher energy than the averge, so even in a classical framework we expect the portion of the packet that crosses the barrier to be non-zero. However in the quantum mechanical context we expect the fraction of the packet that crosses the barrier to be greater. We prove it by calculating the probability of the state of reaching the region x>0 by according to both points of view.

First we calculate the average energy of the state

```
classicE= k_0^2/(2) + V(11.25) %almost the whole energy is due to kinE
```

```
classicE = 50.0525
```

```
V_0=V(0) %energy in the centre of the barrier (x=0)
```

```
V_0 = 655.6331
```

Ψ decomposition over the base of H

The classical probability of crossing the barrier is calculated by projecting the state on the basis of the Hamiltonian, interpreting the state as a gaussian distribution of energy

```
W=@(x)((a.*x).^2 - shift^2).^2/24;
[H,~,Htri] = hamiltonian1D_mod(N,a,V,'DBC');
[Phi,E] = eig(H);
E=diag(E);

projection_Psi = abs(Phi'*psi0).^2 ;
disp('classic trasmission probability')
```

```
classic trasmission probability
```

```
P_classic=sum(projection_Psi(E>V_0))^2
```

```
P_classic = 0.0115
```

Quantum tunneling measurement

According to quantum mechanics the probability for the wave packet to cross the potential hill (in x=0) is obtained as the probability of the time evolution of the state

```
%plot(x,psi)
disp('probability of crossing the state')
```

```
probability of crossing the state
```

```
P_quant=norm(psi(x>0))^2
```

```
P_quant = 0.1045
```

Let's verify that Unitariety is conserved after the transformation

```
norm(psi)
```

```
ans = 1.0000
```

As we can see the probability of crossing the barrier in a classical framework is way lower than the quantum-mechanics probability, gained as the integral of the intern product between $\Psi \text{ and } \Psi^*$.

```
disp('Tunnel effect')
```

```
Tunnel effect
```

```
P_quant-P_classic
```

```
ans = 0.0930
```

In this simulation on a brief interval of time, small enough to interrupt the it before portions of the state begin to interfeere with each other.

Time evolution - Direct method

The direct method to compute the time evolution of a state consists in the direct product $U(\tau)|\Psi\rangle = e^{-\mathrm{i}\mathrm{H}\tau}|\Psi\rangle$

```
s=3e4; %reducing plot scale factor for the state
Chi = psi0;
U = expm(-1i*H*tau);
```

```
tic;
for j=1:nt
    Chi = U*Chi;
    %if mod(j,10) == 0
    %    hf.YData = s*abs(psi).^2;
    %    ht.String = sprintf('t = %-5.2f',j*tau);
    %    drawnow;
    %end
end
toc;
```

```
Elapsed time is 4.245618 seconds.
```

Accuracy

```
disp('complex Chi square between the two methods')
```

```
complex Chi square between the two methods
```

```
disp(sum((Chi-psi).^2)/length(psi));
```

```
   2.2098e-13 + 7.5930e-13i
```

It is clear that the operator splitting technique is faster than the direct method.

Now we can compare the probability of quantum tunneling with both methods to check the accuracy of operator splitting.

```
norm(Chi)^2-norm(psi)^2
```

```
ans = -4.8850e-14
```

We find out that the difference between the two results is negligible: operator splitting is a valid algorithm to solve the time dependent Schrodinger equation.