Teaching wave mechanics with Matlab

To avoid any misunderstanding, let's make it clear that this is not a place where one can learn about professional software devoted to a numerical approach in atomic or molecular physics. For this aim you should look elsewhere for implementations of quantum MonteCarlo, like *Car-Parrinello*. Here instead you will find ideas and techniques useful for teaching elementary wave mechanics to undergraduates. This doesn't mean that our methods cannot lead to original research, they actually originated from research activity, specifically looking for the impact of background geometry on quantum spectra[1], but they are mostly useful for pedagogical applications. You'll find here a basic technique, essentially Feynman Path integral, which allows to study the evolution of wave packets according to Schroedinger's equation, in any given energy potential and display the effect of diffraction, interference, energy barrier penetration (tunnel effect). The calculation of energy spectra for charged particles in external magnetic fields, the nice phenomenon of Landau Levels and Quantum Hall Effect can be approached with our techniques.

---

[1] C. Destri, P. Maraner, and E. Onofri, *Nuovo Cimento A*, **107**, 237 (1994).
P.Maraner, ,E.Onofri and G.P. Tecchiolli, *Spectral methods in computational quantum mechanics, J.Comput.Appl.Math., 37, (1991) 209-219.*

The basic idea, known as "*splitting method*"or "*Leapfrog algorithm*", goes back to Isaac Newton! His proof of the Law of Areas, aka angular momentum conservation, introduces a trick: imagine that the planet evolves inertially for an infinitesimal time Δt as a free particle - hence no attraction from the Sun, hence for another interval Δt the position stays fixed but momentum gets an impulse $\Delta p = F\Delta t$, where F is directed towards the Sun according to His Law. If the interval is small enough the result is equivalent to a correct solution of the equation of motion. See Newton's Principia[2]! Now, the same idea can be exported to quantum mechanics, This translates to the well known Trotter's formula (originally invented by Sophus Lie in the context of continuous groups), namely the quantum evolution given by the unitary operator $U(t) = \exp\{-it(p^2/2m + V(q))\}$ can be approximated with arbitrary accuracy choosing an infinitesimal interval of time *t/n* and computing $U(t) \approx \left(\exp\{-it/n\, p^2/2m\}\ \exp\{-it/n\, V(q)\}\right)^n$. The advantage is twofold, with respect to other numerical recipes: each exponential can be computed *exactly (i.e. to machine accuracy)* and the result is by construction a *unitary operator,* hence there is no loss of probability along the way. Energy is conserved only approximately, namely $n\, \mathcal{O}(\Delta t/n)^2$, but this can be improved at the expense of speed. The crucial ingredient which allows to compute very efficiently the first exponential $\exp\{-i\Delta t p^2/2m\}$ is represented by the fast Fourier transform. We go to Fourier space by Fourier, then the free evolution driven by $p^2/2m$ is simply a multiplication by a phase factor and the inverse Fourier takes us back to position space, where the exponential

[2] For instance on gallica.bnf.fr

$\exp\{-i\,\Delta t\,V(q)\}$ is also a pure phase factor. The idea is due to M.D. Feit, J.A.Fleck and A. Steiger[3].

On your personal computer the method can be implemented using Matlab to study quantum dynamics for scalar particles in one-two and three dimensions. You will find Matlab codes in this repository for a suite of problems, but the good idea is to grasp the essential idea and to try to build yourselves the program, why, you could do better than us!

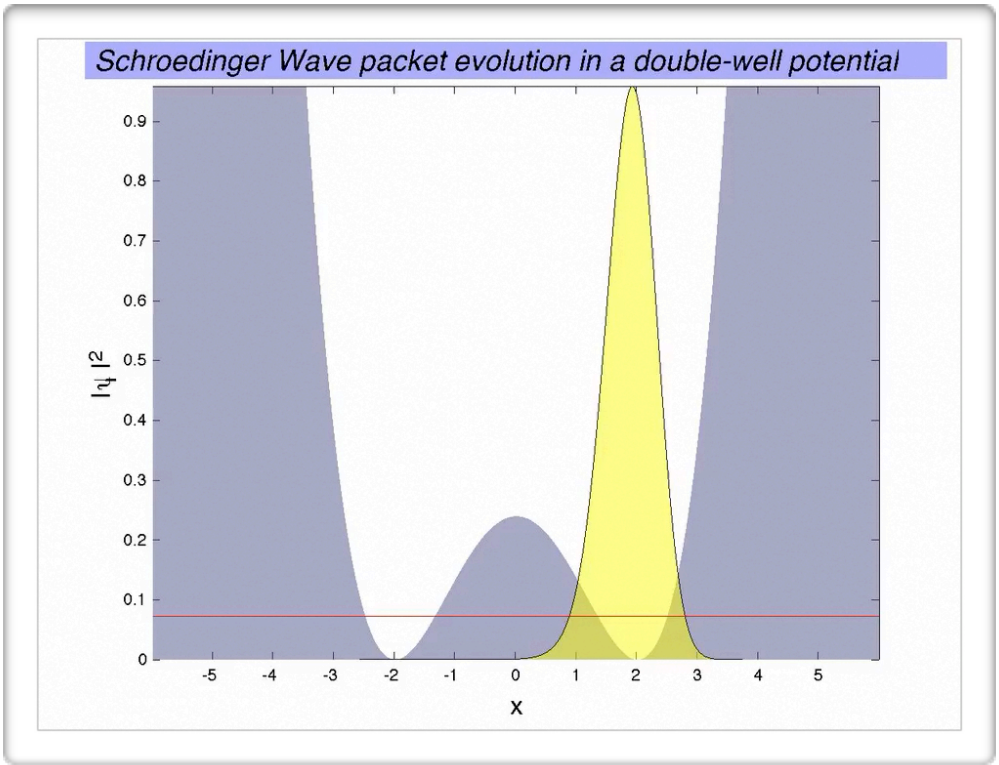
The technique can also be used to estimate the energy spectrum: if you compute the time evolution $\psi(t) = U(t)\,\psi(0)$ then the spectrum is encoded in the wave function. You can extract the spectrum by Fourier analysing the overlap $\langle\psi(0)\,|\,\psi(t)\rangle$ which is given by

$$\sum_n |\langle\psi(0)|E_n\rangle|^2\,\exp\{-i\,t\,E_n\}$$

This was the proposal in the original reference (3). At present this is not the best choice, since we can compute the spectrum by other "sparse" methods much more efficient (Arnoldi method), as you may find elsewhere in this blog.

[3] M.D. Feit, J.A. Fleck Jr and A. Steiger, J. Comput. Phys. 47 (1982) 412-433.

We suggest to start with two examples - *"doublewell.m"* and "*wms2.m*". The first program displays the evolution of a quantum particle in a potential exhibiting two classical vacua, namely $V(x) = V_0 (x^2 - a^2)^2$. Let the particle be located as a Gaussian packet around $x=a$ at $t=0$; quantum evolution makes it evolve oscillating around $x=a$ and we see its leaking to the left region



around $x = -a$ *even if its energy is less than* $V_0 a^2$ due to the tunnel effect. This is a simplified model of what really happens in the ammonia molecule NH_3 .

Now let's look at the code in detail. You may conveniently keep the code under your sight with an editor, here we give some essential comments. The function interface is very concise…

```
function setup=doublewell(setup)
```

The interaction with the user is through a setup file. If you start from scratch this can be empty and a default will be provided; it is then saved with your choices in order to be able to restart with the same initial setup or a variation thereof. The setub file contains all physical parameters *mass, momentum, width of the wave packet,* and other "technical" parameters which define the computing environment *box size, grid size, evolution time, etc.*. Then come the definition of the position grid (here 1-dimensional)

```
dx  = 2*L/N
 x   = -L*(1-1/N) : dx : L*(1-1/N);
```

and the momentum space grid

```
k = fftshift(pi*(-N/2:(N/2-1))/L);
```

Then we define the potential energy

```
V = V0 * (1-(x/omega).^2).^2;
```

The spitting algorithm requires the two phase factors $\exp\{-i\Delta t p^2/2m\}$ and $\exp\{-i\,\Delta t\,V(q)\}$, thus

```
U = exp(-i*tau*V);  U2 = exp(-0.5i*tau*V);
W = exp(-0.5i*k2/mass*tau);
```

U2, a half step evolution, is used to build a symmetric algorithm, as we can see in the full listing. The initial wave packet is built as a normalized Gaussian, centered around one minimum of the potential

```
psi = exp(-(x-x0).^2/4/sigma+i*mom*x)/2*pi*sigma).^(1/4);
```

The evolution is given by a loop over the number of time steps, each consisting of the application of the phase factors to the wave

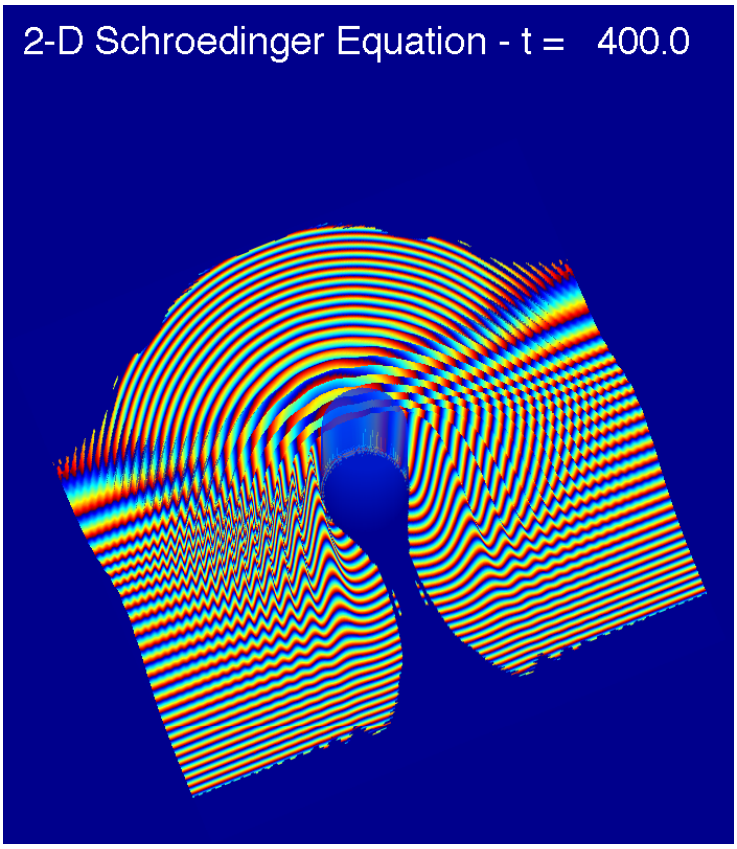
function alternatevily in position and in momentum space, just one line

```
psi = U.*ifft(fft(psi).*W);
```

but it may be clearer by unfolding it to

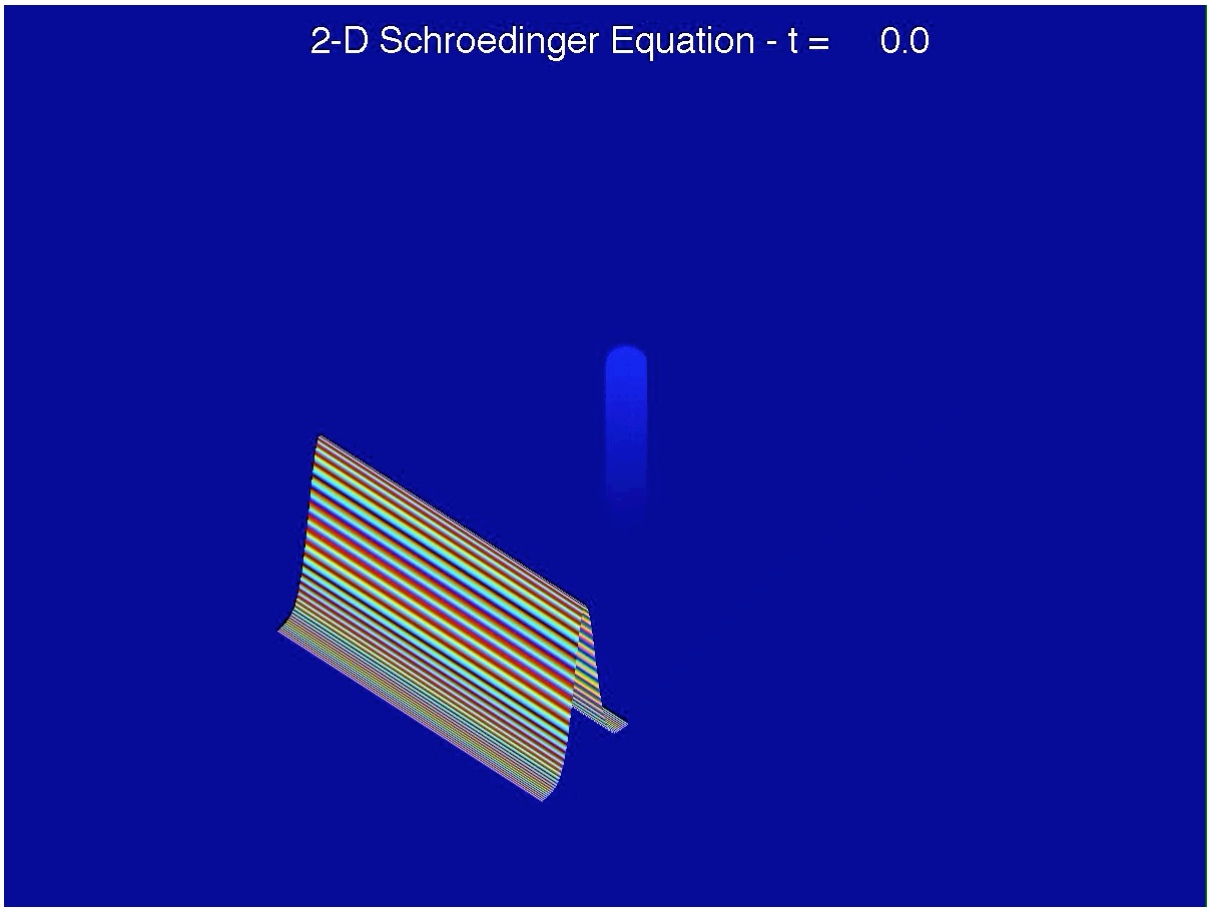
```
phi = fft(psi); % go to momentum space
phi = W.*phi;       % apply W=exp(-i dt p^2)
psi = ifft(phi);% back to position space
psi = U.*psi;    % apply U = exp(-i dt V(x))
```

In this loop we spend most of the computing time. The rest of the code is devoted to the graphical display of the probability density $\rho(x,t) = |\psi(x,t)|^2$. An option lets us to save the snapshots in order to produce a stand alone video clip. Let's skip the details.



The second example consists in the evolution of a wave packet in two-dimensions and it can be used to display the phenomena of diffraction and interference typical of wave mechanics. In the multidimensional case we have to work a bit more in defining the position grid and momentum grid. This can be easily done using Matlab's built-in routines *meshgrid* or *ndgrid*. The core of the program is essentially identical, given we employ the two-dimensional version of the fast Fourier tranform *fft2* and *ifft2*. The display is organised to give both the probability density and the phase: this latter is rendered by a color code which is linked to the phase. In this way one can check the difference between *phase velocity* and *group velocity!* Here we have a plane wave packet scattering around a potential barrier and we can see the back scattered circular wave and the main packet continuing in the original direction.

A video clip with about this problem can be found as "*thebigone.mov*" in the file depository.

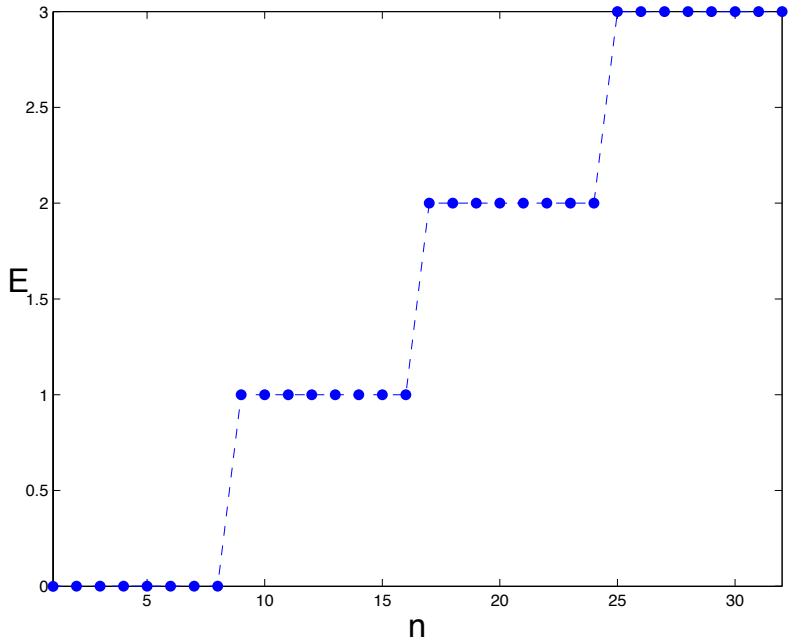


Landau levels

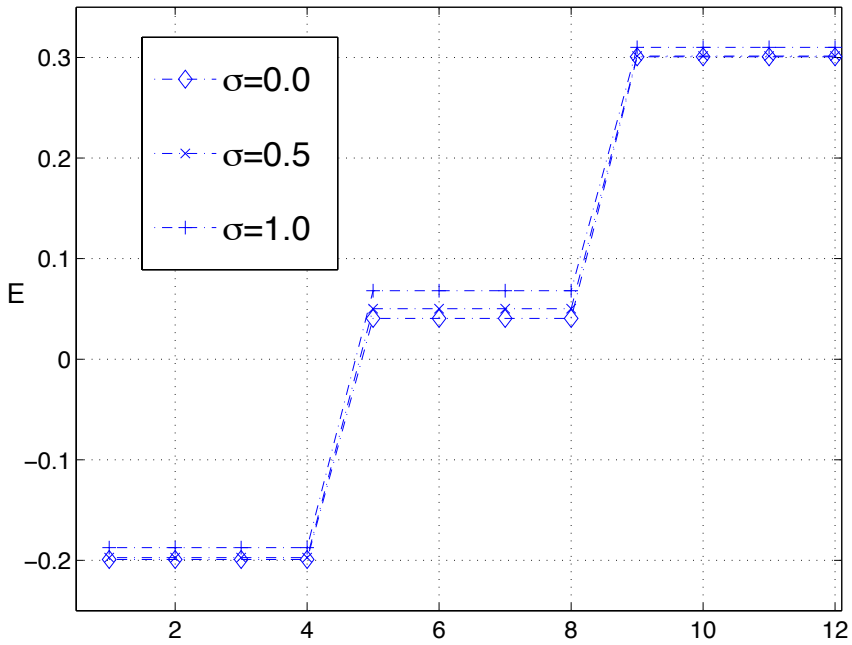
Now we introduce another elementary application of the splitting technique which has a distinguished character: Landau Levels on the computer. The subject has been for decades a topic in Mathematical Physics, since the 1930 paper by Landau, but in recent years it has been reconsidered or its phenomenological relevance[4]. The problem consists in computing the energy spectrum for a charged particle in two dimensions subject to a transverse uniform magnetic field. The problem allows for a complete analytic solution (Landau), but the availability of a precise numerical computation make it possible to estimate the effect of various perturbation, which is not always possible analytically. Our method consists in representing momenta using the trick to go in momentum space via *fft*, however this implies that we are working with periodic boundary conditions hence the particle lives on a torus. If the size of the torus is large enough this has little impact on the physics of the problem, but the interesting features of the problem manifest themselves in the opposite case, when we insist on having to do with a particle on a torus and a transversal magnetic field; since a strictly solenoidal field must have zero flux this means that we are actually studying a field generated by a suitable magnetic charge and this must be in accord with Dirac's quantization condition - hence the flux is quantized. The energy levels turn out to have a degeneracy exactly given by the quantized flux! We can then experiment what happens in presence of various

[4] Int.J.Theoret.Phys. 40(2) 537, 2001; Int.J.ModernPhys.C, 2008.

perturbations. Details can be found in the two references; see also Ref. (5). Matlab code can be found in the blog repository under the name *LL2.m*.



An example of Landau spectrum with monopole charge 8.



[5] P.Maraner, G.P.Tecchiolli and E.O., *Spectral methods in computational quantum mechanics*, J. Comput. Appl. Math., 37 (1991).

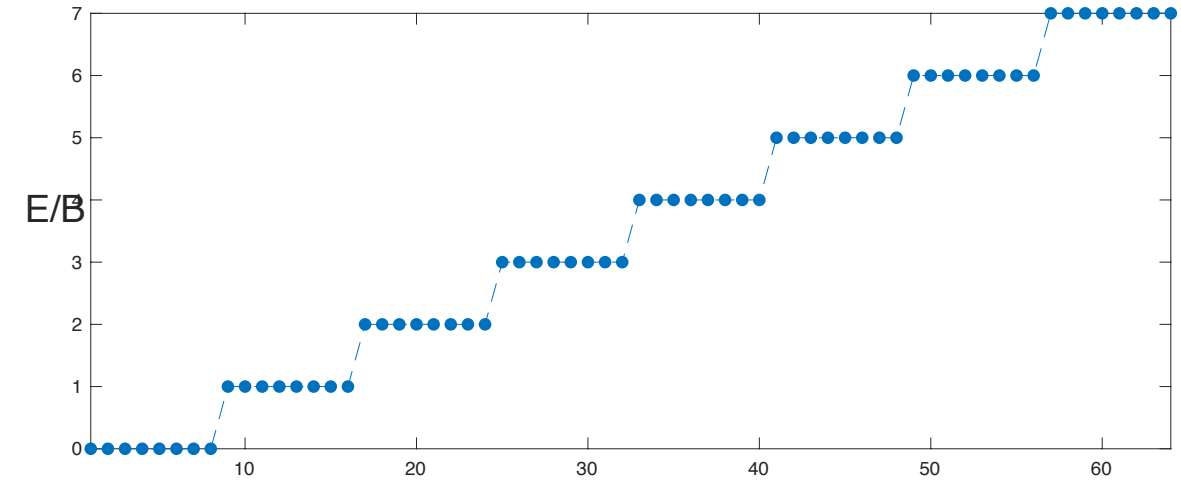
The previous plot shows that u*nder a periodic perturbation the Landau levels are rather stable,* which is important since in real materials impurities are always present. This appears to be hard to prove analytically.

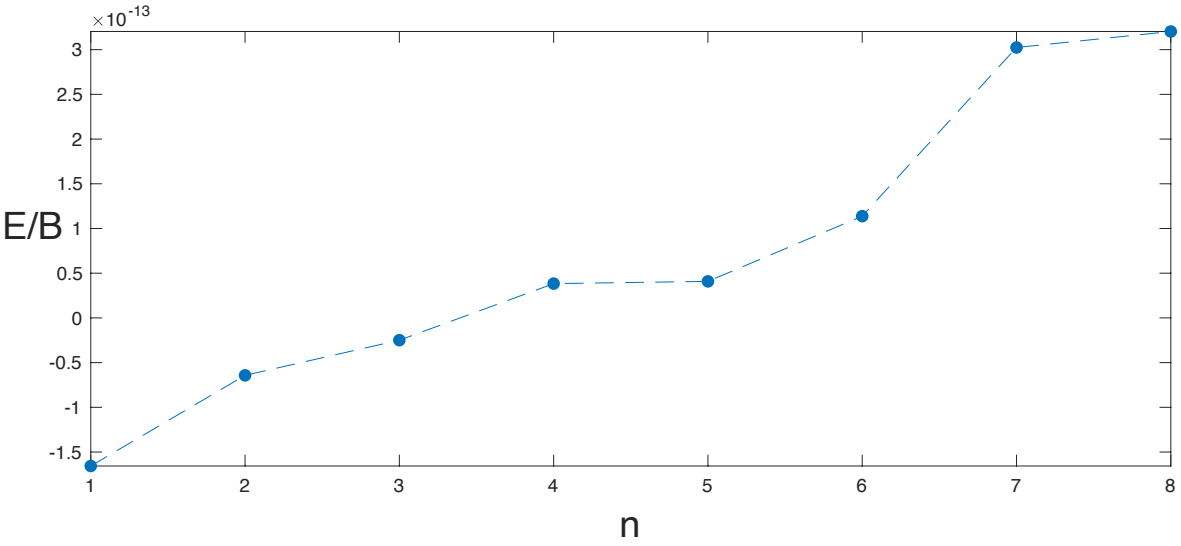
The essential features of the program are the following:

1. we do not use a discretisation to represent the momentum operators, rather we resort to the spectral representation based on the fast Fourier transform.
2. we take into account that the wave function for a charged particle on a compact manifold (here the torus) subject to a transversal magnetic field is not just a periodic function on the torus, rather it is a section of the line bundle built according to the rules of quantum gauge theories. This obliges us to introduce a correction with a phase factor *before* taking the Fourier transform. Details can be found in the first references.
3. The spectrum is computed using the matlab routine ***eigs*** which implements the *Krylov-Schur* algorithm[6]: it allows to define the Hamiltonian operator through a subroutine instead of giving explicitly its matrix representation. The accuracy of the method is remarkable. See the following plot where the degeneracy of the levels is reproduced to the required accuracy 10^{-12}.

[6] Stewart, G.W. "*A Krylov-Schur Algorithm for Large Eigenproblems.*" SIAM Journal of Matrix Analysis and Applications. Vol. 23, Issue 3, 2001, pp. 601–614.

The relevant code, to be found in the archive, is called *LandauMathieu.m*.





Bosonic operators

A good knowledge of Dirac's creation-annihilations operators is required to all students in elementary quantum mechanics. This requires some proficiency in algebraic manipulations for non-commuting operators. Typical academic exercises are the calculation of perturbed energy level for a Hamiltonian of the kind

$$H = \hbar\omega\, a^{\dagger} a + \lambda(a + a\dagger)^4$$

or multidimensional Hamiltonians like

$$H = \hbar\omega(a_1^{\dagger} a_1 + a_2^{\dagger} a_2) + \lambda\,(a_1^{\dagger} a_2 + a_2^{\dagger} a_1)$$

Such problems can be solved rather easily using a symbolic language like Mathematica or form, here however we discuss how we can approach these problems via Matlab achieving high accuracy. The crucial elements in order to represent Bosonic operators in an efficient way are 1) sparse matrices, 2) Kronecker products. Sparse matrices allow for large matrix dimensions and the Kronecker product "kron" allows to build multidimensional bosonic operators starting from the one diimensional ones. The simple one-dimensional operators can be defined like this

```
%----Creation/annihilation operators----
function [a,ad] = boson(B)
D  = (0:B)'; % diagonal mat.elem. (column vector)
a  = spdiags(sqrt(D), 1, B, B); % creation operator
ad = a';
```

The built-in matlab routine **spdiags** defines a sparse matrix built by specifying its diagonals, in this case the upper diagonal, at distance 1 from the main diagonal. The advantage of using sparse matrices consists in saving the memory required, which grows linearly with the matrix dimension, and in speed of the arithmetic routines. In the first example we may study the harmonic oscillator in two dimensions as implemented in the routine **Boson2D.m;** various choices of the perturbation are listed in the code but can easily modified by yourself. Notice that when the perturbation is absent we can check the accuracy of the algorithm since the spectrum is known exactly: a call

```
E = Boson2D('1',0,100,64);
```

returns the known spectrum with a maximum error $\mathcal{O}(10^{-14})$. The big difference here is that a full matrix describing the 2D bosonic operators would require $\mathcal{O}(N^4)$ words in memory, here N=100, hence 10^8 words, whereas the correspondig sparse matrix occupies only 10^4 words, a mere 200kBy! The difference is obviously even more relevant for 3 or 4 dimensions.

For the 3D example

$$H = \hbar\omega\,(a_1^\dagger a_1 + a_2^\dagger a_2 + a_3^\dagger a_3) + \lambda(a_1^\dagger a_2 + a_2^\dagger a_3 + a_3^\dagger a_1)$$

the code gives the perturbed spectrum in a context of degenerate energy levels; here an exact calculation is possible and you may check the accuracy of the matlab routines, which would be difficult to reach by other techniques.

The code ***Boson1D.m*** and others present in the distribution can be modified to allow for multiple precision calculations, e.g. using *Advanpix* toolbox. Thus we can

appreciate the accuracy of the Lanczos-Arnoldi methods. For instance the ground state of the anharmonic oscillator which is known to have an asymptotic expansion with leading terms

$$E_0 \sim \frac{3}{4}\lambda - \frac{21}{8}\lambda^2 + \frac{333}{16}\lambda^3 - 30885/128\,\lambda^4 + \ldots$$

can be used to check the accuracy with excellent results, e.g $O(10^{-12})$ for $\lambda = 0.001$. The usage of multi-precision routines can be applied to higher dimensional codes **`Boson?D.m`**, and is left as an exercise.