OPTI 571L Lab 1: Basic MATLAB Techniques for Quantum Mechanics

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Matrices play a fundamental role in quantum theory both as representations of operators in matrix mechanics and also in the form of eigenvalue problems to determine the stationary states and allowed energies for a system. MATLAB is an ideal tool for the numerical solution of eigenvalue problems and we explore this capability in this lab. As a first example we consider two classical coupled oscillators which permits comparison of analytic and numerical solutions of the eigenvalue problem, and also the consideration of simple dynamics. The second example involves the extension to an array or lattice of coupled oscillators. Finally we show how to employ these ideas in MATLAB to calculate the eigenmodes and energies of a particle in a potential well and wave packet dynamics.

Keywords: Matrices, eigensolutions, coupled oscillators, numerical solution of the one-dimensional Schrödinger equation, wavepacket dynamics, anharmonic and double-well potentials.

I. EIGENVALUE PROBLEMS IN MATLAB

MATLAB has a powerful eigenvalue solver called `eigs` (or another called `eig`) that determines the eigenvalues and eigenvectors of an $(N \times N)$ matrix that we denote M. You should look up the documentation for `eigs` using the help command in MATLAB and become familiar with it (you can use another solver but you should describe it if you choose to do so). Basically, [V,D] = `eigs`(M,N) returns a $(N \times N)$ diagonal matrix D of the N eigenvalues and a $(N \times N)$ matrix V whose columns are the corresponding eigenvectors. Denoting the eigenvalues $\lambda_j = D_{jj}$ with $j = 1, 2, \ldots N$, and writing $V = [\bar{v}_1, \bar{v}_2, \ldots, \bar{v}_N]$, with the column vectors $\bar{v}_j$ denoting the eigenvectors, the underlying eigenvalue problem may be written as

$$\lambda_j \bar{v}_j = M \bar{v}_j. \tag{1}$$

Here we use j to label the eigensolutions, whereas we use μ to label the components of a given eigenvector $\bar{v} = col[v_1, v_2, \ldots, v_\mu, \ldots, v_N]$. For a Hermitian matrix M and non-degenerate eigenvalues the calculated eigenvectors form a complete orthonormal set of basis vectors

$$\bar{v}_j^\dagger \cdot \bar{v}_k = \delta_{jk}, \tag{2}$$

with † signifying an adjoint (transpose and conjugate). Then an arbitrary vector $\bar{v}$ can be expanded in terms of the eigenvectors as

$$\bar{v} = \sum_{j=1}^{N} c_j \bar{v}_j, \quad c_j = \bar{v}_j^\dagger \cdot \bar{v}, \tag{3}$$

with expansion coefficients c_j. As an example consider the matrix

$$M = \begin{pmatrix} 1 & -0.1 \\ -0.1 & 1 \end{pmatrix}. \tag{4}$$

The results below will be of use later but there is no need to turn in solutions for parts (a-d) below, they are included in case you need a reminder of how eigenvalues and vectors are calculated.

(a) Find the eigenvectors and eigenvalues analytically for this problem.

(b) Next write a code to find and output the eigenvectors and eigenvalues using `eigs` and compare against the analytic solutions. Note any differences that might arise beyond simple numerical roundoff.

(c) Building on your code from part (b) numerically demonstrate that the eigenvectors from part (b) are orthonormal.

(d) Find an expression for the column vector $\bar{c}$ of expansion coefficients for an arbitrary vector $\bar{v}$ that employs the output from `eigs`.

A. Two-dimensional example

As a first example of the problem at hand we consider two simple harmonic oscillators with coordinates $x_1(t)$ and $x_2(t)$ and natural frequency ω, that are weakly coupled

$$\begin{aligned} \frac{d^2x_1}{dt^2} &= -\omega^2 x_1 + \kappa x_2, \\ \frac{d^2x_2}{dt^2} &= -\omega^2 x_2 + \kappa x_1, \end{aligned} \tag{5}$$

where κ characterizes the strength of the coupling. These equations are appropriate for two coupled pendula with small displacements, or more generally two oscillators in close enough spatial proximity that they are coupled. Having a physical system in mind can help intuit the results obtained.

(a) The above pair of second-order differential equations may be written as a system of first-order differential equations using $R_{1,3} = x_{1,2}, R_{2,4} = \frac{dx_{1,2}}{dt}$ giving

$$\frac{d}{dt}\begin{pmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{pmatrix} = \frac{d\bar{R}}{dt} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -\omega^2 & 0 & \kappa & 0 \\ 0 & 0 & 0 & 1 \\ \kappa & 0 & -\omega^2 & 0 \end{pmatrix}\begin{pmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{pmatrix} = A\bar{R}. \tag{6}$$

The solution of this equation may be written as $\bar{R}(t) = e^{At}\bar{R}(0)$. As a numerical example for the remainder of this problem we choose $\omega = 1, \kappa = 0.1$. For initial excitation of only one oscillator, $x_1(0) = R_1(0) = 1, x_2(0) = R_3(0) = 0, R_{2,4}(0) = 0$ use the information above to solve for and plot $x_{1,2}(t)$ over the range $t = [0, 62.7]$ using 1000 time points. (For this the MATLAB routine `expm` will prove useful.) This example illustrates the utility of matrix methods for solving systems of ordinary differential equations, and is easily extended to include time-dependent coefficients and nonlinearity. Here we stress the utility of matrix methods but another approach is to use the MATLAB routines for systems of ordinary differential equations such as `ode23` or `ode45`.

(b) By seeking time-harmonic solutions of Eqs. (5) of frequency Ω and the specific form

$$\bar{x}(t) = \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} = \cos(\Omega t)\bar{v}, \tag{7}$$

show that one obtains an eigenvalue problem of the form in Eq. (1). We choose $\omega = 1, \kappa = 0.1$ so that you have the corresponding eigenvalues and eigenvectors already from problem (a) of Sec. 2.

(c) A general initial condition can be written as a sum of the eigenvectors

$$\bar{x}(0) = \sum_{j=1}^{2} c_j \bar{v}_j. \tag{8}$$

For initial excitation of only one oscillator, $x_1(0) = 1, x_2(0) = 0$, use your results from part (b) to find a solution for the time-dependent positions $x_{1,2}(t)$.

(d) Compare your analytic results from part (c) with the numerical results from part (a), and also with your expectations of how this system should behave physically. This example is meant to illustrate the utility of eigensolutions as a basis for the solution of systems of equations. In this case one uses a superposition of the eigensolutions to represent a general solution.

The analysis performed here is a prototype for the dynamics of two-state systems including Rabi-flopping in a laser driven two-level atom, the quantum dynamics of a qubit, and Josephson oscillations between Bose-Einstein condensates.

B. N-dimensional example

Here we generalize to the case of an array or lattice of N simple harmonic oscillators with coordinates $x_\mu(t)$ that are weakly coupled

$$\frac{d^2x_\mu}{dt^2} = -\omega_\mu^2 x_\mu + \kappa x_{\mu+1} + \kappa x_{\mu-1}, \quad \mu = 1, 2, \ldots, N, \tag{9}$$

where ω_μ is the natural frequency of the oscillator labeled μ. Here we have used nearest-neighbor-coupling, so that oscillator μ is coupled to $(\mu \pm 1)$. There is an issue of boundary conditions for $\mu = 1, N$, in particular how do we assign $x_0(t)$ and $x_{N+1}(t)$ in evaluating the right-hand-side of Eq. (9)? For natural boundary conditions, as in our previous example with $N = 2$, one enforces

$$x_0(t) = x_{N+1}(t) = 0, \tag{10}$$

whereas for periodic, or von Karman, boundary conditions one imposes

$$x_0(t) = x_N(t), \quad x_{N+1}(t) = x_1(t). \tag{11}$$

For the case of natural boundary conditions we may consider a linear array of pendula, whereas for the periodic boundary conditions we may imagine the same pendula arranged on a circle.

(a) Show analytically that seeking time-harmonic solutions of frequency Ω of the form $\bar{x}(t) = \cos(\Omega t)\bar{v}$ with natural boundary conditions leads to an eigenvalue problem of the form in Eq. (1) with

$$M_{\mu,\nu} = \omega_\mu^2 \delta_{\mu,\nu} - \kappa[\delta_{\mu,\nu+1} + \delta_{\mu,\nu-1}]. \tag{12}$$

(b) For the case with $N = 41$ and $\omega_\mu = 1, \kappa = 0.2$ numerically find the eigenvectors and eigenvalues, and plot the eigenvector components x_μ as a function of μ for the four smallest eigenvalues.

(c) Do these eigenvectors bear any resemblance to solutions of a problem you have encountered in quantum theory? Highlight any features that are shared with the quantum problem.

(d) As before a general initial condition can be written as a sum of the eigenvectors

$$\bar{x}(0) = \sum_{j=1}^{N} c_j \bar{v}_j. \tag{13}$$

Consider initial conditions of the form $(\bar{x}(0))_\mu = \exp(-(\mu-21)^2/\sigma), \mu = 1, 2 \ldots, N$. Plot $x_{21}(t)$ versus t for the two cases $\sigma = 10, 100$ over the time range $t = [0, 1094]$ using 10000 time points, and plot $x_\mu(t)$ versus μ for $t = 0, 547, 1094$.

(e) For one of the two cases in part (d) the initial wave is almost reconstructed at $t = 1094$, whereas for the other case the evolution is more complicated. By examining the *mode spectrum* $|c_j|$ versus mode index j for the two cases build a rationale for the difference between the two cases.

(f) Based on your rationale from part (e) provide an approximation to the observed reconstruction time $t = 1094$ in terms of the eigenvalues, and also give an explanation of the profile $x_\mu(t)$ for $t = 547$.

The analysis performed here is a prototype for lattice dynamics including phonons in solids, Josephson oscillations in arrays of Bose-Einstein condensates, and mode-locking of matter waves. The key being that the eigenvectors are a natural basis for the exploration of lattice dynamics.

II. QUANTUM EIGENMODES OF A POTENTIAL

In this section we apply the ideas of the previous sections to finding the quantum eigenmodes of a time-independent potential. We already have the machinery for this and it remains to show how to apply this to the Schrödinger equation. We treat the 1D quantum harmonic oscillator as this has an analytic solution to check against.

A. Schrödinger equation

We start from the one-dimensional time-dependent Schrödinger equation for the wave function $\Psi(z,t)$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial z^2} + V(z)\Psi, \tag{14}$$

with time-independent potential $V(z)$ [1]. The eigenmodes follow from the replacement $\Psi(z,t) = \psi(z)e^{-iEt/\hbar}$ giving the time-independent Schrödinger equation

$$E_j\psi_j(z) = -\frac{\hbar^2}{2m}\frac{d^2\psi_j}{dz^2} + V(z)\psi_j, \quad j = 0,1,2,\ldots \tag{15}$$

The eigenmodes form a complete orthonormal set of expansion functions meaning that a general wave packet may be written as

$$\Psi(z,t) = \sum_{j=0}^{\infty} c_j\psi_j(z)e^{-iE_jt/\hbar}, \tag{16}$$

where the expansion coefficients are

$$c_j = \int_{-\infty}^{\infty} dz\ \psi_j^*(z)\Psi(z,0). \tag{17}$$

For the case of a harmonic oscillator with $V(z) = \frac{1}{2}m\omega^2z^2$ the eigenvalues of this equation are $E_j = \hbar\omega(j+1/2)$ and the eigenvectors are the Hermite-Gaussian functions

$$\psi_j(z) = \mathcal{N}_jH_j(z/z_0)e^{-z^2/2z_0^2}, \tag{18}$$

with $\mathcal{N}_j$ normalization constants, and $H_0(s) = 1$ for the ground state, $H_1(s) = 2s$, for the first excited state, and so on [1]. In particular, the width of the Gaussian ground state is characterized by $z_0 = \sqrt{\hbar/m\omega}$, and the spatial extent of higher modes scales as $z_j = z_0\sqrt{2j+1}$.

B. Discretization of the Schrödinger equation

To approach the problem numerically we need to introduce a discrete numerical grid along z with N equally spaced points

$$z_\mu = -\frac{z_{max}}{2} + (\mu-1)\Delta z, \quad \mu = 1,2,\ldots,N \tag{19}$$

with z_{max} the width of the numerical grid that is symmetric around $z = 0$, and $\Delta z = z_{max}/(N-1)$ the spacing between grid points. Given the ground state width z_0, in general we require $\Delta z << z_0$ and $z_{max} >> z_0$.

The wave function at the grid point z_μ is labelled $\psi(z_\mu) = \psi_\mu$, and similarly for the potential $V(z_\mu) = V_\mu$. Then on the discrete spatial grid the second-order spatial derivative may be evaluated using the three-point approximation

$$\frac{d^2\psi}{dz^2} \to \frac{(\psi_{\mu+1} - 2\psi_\mu + \psi_{\mu-1})}{\Delta z^2} \tag{20}$$

(a) Using the above information, and employing natural boundary conditions at the edge of the spatial domain, show that the eigenmodes follow from the eigenvalue problem

$$E_j\bar{\psi}_j = H\bar{\psi}_j, \tag{21}$$

with discrete matrix form of the Hamiltonian

$$H_{\mu,\nu} = \left[V_\mu + \frac{\hbar^2}{m\Delta z^2}\right]\delta_{\mu,\nu} - \frac{\hbar^2}{2m\Delta z^2}[\delta_{\mu,\nu+1} + \delta_{\mu,\nu-1}]. \tag{22}$$

(b) The MATLAB routine `eigs` provides normalized eigenvectors obeying $\sum_\mu |v_\mu|^2 = 1$. How can the output from `eigs` be used to provide discrete approximations to the eigenmodes ψ_j with normalization appropriate to the wave function?

Thus the continuous Schrödinger equation can be approximated on a discrete grid as a lattice problem represented by a matrix which lends itself to numerical solution of the eigenmodes using MATLAB.

C. Quantum harmonic oscillator

(a) Show that for the case of the harmonic oscillator the Hamiltonian matrix takes the form

$$h_{\mu,\nu} = \frac{H_{\mu,\nu}}{\hbar\omega} = \left[\frac{1}{2}(z_\mu/z_0)^2 + (z_0/\Delta z)^2\right]\delta_{\mu,\nu} - \frac{1}{2}(z_0/\Delta z)^2[\delta_{\mu,\nu+1} + \delta_{\mu,\nu-1}]. \quad (23)$$

For concreteness we consider parameters for which $z_0 = 1$ μm.

(b) By diagonalizing the matrix h using MATLAB solve for the eigenvalues and eigenmodes of the quantum harmonic oscillator. For this you will need to choose values for z_{max} and N and some experimentation will be needed on your part - you may want to revisit your calculations as you gain experience on choosing a grid. For example, $z_0 = 1$ μm sets the spatial scale of the ground state and we would like enough points to spatially resolve this, say 10 points to start with. Then if we set $z_{max} = 4z_0 = 4$ μm as the grid width then we should choose $N = 40$.

(c) In general the grid spacing Δz used should be small enough that that the eigenmodes are well sampled. The ground state width is z_0 so we need $(\Delta z/z_0) << 1$. Check that the ten lowest energy eigenvalues obtained from the Hamiltonian h agree to a reasonable precision with the analytic values. Use this to select parameters for your grid.

(d) By plotting the *normalized* eigenmodes ψ_μ versus z_μ on the discrete grid compare your results with the known exact solutions for the first four eigenmodes.

(e) For the quantum harmonic oscillator the highest mode that can be captured with a given grid may be estimated as follows: The mode size scales as $z_j = z_0\sqrt{2j+1}$ so our lattice approximation breaks down for $z_j \geq z_{max}/2$, or $j > j_{max} \simeq (z_{max}/2\sqrt{2}z_0)^2$. Check this estimate by plotting the ratio

$$r_j = \frac{\epsilon_j - (j+1/2)}{(j+1/2)}, \quad j = 0, 1, ...N \quad (24)$$

as a function of (j/j_{max}), with ϵ_j the eigenvalues of h. This ratio represents the fractional change in the numerical eigenvalues compared to the exact values.

The message is that for a given discretization one should not consider modes with $j > j_{max}$. In particular, if one is consider wave packet dynamics the *mode spectrum* $|c_j|$ versus j should not have significant population above or in the near vicinity of j_{max}.

Further exploration: Suggestions include the Pöschl-Teller potential which also has exact solutions, the Morse potential which is a model for molecular vibrations, or finding the eigenmodes and eigenvalues of periodic potentials. The final example requires implementation of periodic boundary conditions and has application in atom trapping in lattices and also electron states in crystals.

D. Anharmonic oscillator

To start this problem we consider some quantum dynamics of the harmonic oscillator. In particular you will need to use the general expression (16) for a wave packet in terms of the modes in combination with Eq. (17) for the amplitudes of each mode. You shall therefore be performing a numerical decomposition of the initial wave function into the modes of the system.

(a) Consider the displaced Gaussian $\Psi_\mu(0) = \mathcal{N}_0 e^{-(z_\mu - 2z_0)^2/2z_0^2}$ as the initial condition, with $\mathcal{N}_0$ a normalization constant. By using your results from this section produce a 2D plot of the spatial probability density $|\Psi_\mu(t)|^2$ versus ωt and μ using `imagesc` in the time range $\omega t = [0, 8\pi]$.

(b) Building on part (a) plot the numerically calculated scaled expectation value of the position $(\langle z(t)\rangle/z_0)$ versus ωt, which traces the wave packet centroid, and compare this against the *exact* solution $(\langle z(t)\rangle/z_0) = 2\cos(\omega t)$.

A key property of a quantum harmonic oscillator is that an initial Gaussian as above remains a Gaussian for all time although its parameters, centroid etc., may change with time. This underlies the simple results above. Next we add some anharmonicity to the potential via the replacement in the Hamiltonian (23)

$$V_\mu = \frac{1}{2}(z_\mu/z_0)^2 \to \frac{1}{2}(z_\mu/z_0)^2 + 0.02(z_\mu/z_0)^4, \quad (25)$$

this representing a quartic addition to the harmonic potential.

(c) For the same initial displaced Gaussian as part (a), produce a 2D plot of the probability density $|\Psi_\mu(t)|^2$ versus ωt and z_μ using `imagesc` in the time range $\omega t = [0, 8\pi]$. You shall see that the anharmonicity can produce large changes. The source of these changes is that the anharmonicity changes the eigenvalues and eigenvectors with respect to the harmonic case, and the initial Gaussian can change drastically under time evolution.

(d) Building on part (c) plot the numerically calculated scaled expectation value of the position $(\langle z(t)\rangle/z_0)$ versus $0 < \omega t < 250$ using 1000 time points. You should see that the initial oscillations collapse with

time but revive, at least partially, with time, so that the anharmonicity has a pronounced effect on the long term wave packet dynamics.

The collapse and revival phenomenon seen here appears in the context of matter wave interference [2] and also the Jaynes-Cummings model of a single-mode interacting with a two-level atom [3].

Further exploration: A suggestion is the anharmonic Hamiltonian $H + \alpha H^2$, with H the Hamiltonian for the harmonic oscillator, and α a constant. This case has an exact solution which may be explored in a later module.

E. Double-well potential

As a final problem consider a double-well potential formed by adding a central repulsive Gaussian potential to the Hamiltonian (23) via the replacement

$$V_\mu = \frac{1}{2}(z_\mu/z_0)^2 \to \frac{1}{2}(z_\mu/z_0)^2 + 4e^{-2z_\mu^2/z_0^2}. \qquad (26)$$

If the nature of this potential is unclear you should plot it.

(a) Consider the displaced Gaussian

$$\Psi_\mu(0) = \mathcal{N}_0 e^{-(z_\mu - 1.3z_0)^2/z_0^2}$$

as the initial condition, with $\mathcal{N}_0$ a normalization constant. Produce a two-dimensional plot of density $|\Psi_\mu(t)|^2$ versus z_μ and over the time range $\omega t = [0, 204.6]$ with 1000 time points using the MATLAB plotting routine `imagesc`. You should see periodic exchange between the two wells centered at $z = \pm 1.3 z_0$ due to tunneling with some superposed shuddering of the wave packet due to the fact that the input Gaussian is composed of a few modes of the double well.

(b) Building on part (a) plot the numerically calculated scaled expectation value of the position $(\langle z(t)\rangle/z_0)$ versus ωt, and read of the period of the tunneling oscillations. These oscillations arise from the beating between the two lowest eigenmodes of the double-well potential. Demonstrate that the period you find is in agreement with the results from your eigenmode solver.

The double-well potential is a central paradigm in quantum physics describing situations ranging from atom tunneling to Josephson oscillations in condensed matter [4], for which Josephson won the 1973 Nobel Prize in Physics for work he did as a graduate student in 1962, on which is based the NIST standard for the volt and sensitive SQUID magnetometers.

Further exploration: A suggestion is to study how the tunneling varies with barrier height, and also to allow for an asymmetric double-well.

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