

BIO 5329: PROBLEM SET 4

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Due at the start of class (8 AM) on November 29. Please hand in the analytical problems in class and e-mail the *well-commented* Matlab M-files to me (baker@ccb.wustl.edu) before class.

1. DAMPED VIBRATIONS (20 POINTS)

This problem considers vibrations in a 1-dimensional linear material (think: DNA, etc.) in a viscous medium such that the time evolution is described by

$$(1.1) \quad u_{tt}(x, t) = ku_{xx}(x, t) - 2\gamma u_t(x, t)$$

where $u(x, t)$ is the displacement of the material at time t and position x , k is related to the speed of vibrations in an undamped medium (e.g., a vacuum) and 2γ is related to the friction induced by the viscous medium (the 2 is there to make the problem a bit easier). We'll assume the ends of the linear material are held fixed such that

$$(1.2) \quad u(0, t) = u(L, t) = 0$$

and the “trajectory” begins with the displacement

$$(1.3) \quad u(x, 0) = \frac{x}{L} - \left(\frac{x}{L}\right)^2$$

and zero velocities

$$(1.4) \quad u_t(x, 0) = 0.$$

1.1. **Separation of variables (5 points).** Separate the partial differential equation above into two coupled ODEs: one for the temporal part of the solution $T_\lambda(t)$ and the other for the spatial part of the solution $X_\lambda(x)$, coupled by the parameter λ .

1.2. **Spatial separated solution (5 points).** Solve the spatial part of the problem for $X_\lambda(x)$ using the zero-displacement boundary conditions (Eq. 1.2).

1.3. **Temporal separated solution (5 points).** Solve the temporal part of the problem for $T_\lambda(t)$ using the zero-velocity initial condition (Eq. 1.4).

1.4. **The entire solution (5 points).** Reassemble the global solution $u(x, t)$ using the separated solutions you obtained above and the initial displacement condition (Eq. 1.3). Plot the solutions in Matlab or Mathematica for $\gamma^2 < \pi^2 k/L^2$ and $\gamma^2 \geq \pi^2 k/L^2$. What's different about these two conditions?

2. 1D ELECTROSTATICS AND SOURCE TERMS (20 POINTS)

In what follows, we're going to consider the linearized Poisson-Boltzmann equation

$$(2.1) \quad -\nabla \cdot (\epsilon(x)\nabla u(x)) + \kappa^2(x)u(x) = \rho(x)$$

in a one dimensional system $x \in [0, L]$ where $u(x)$ is the electrostatic potential, $\epsilon(x) \geq 1$ is the dielectric coefficient, $\kappa(x) \geq 0$ is a screening parameter due to aqueous ions, and $\rho(x)$ is a “stationary” charge distribution. Despite the simplified geometry, this equation can be used to generate a reasonable

description of membrane electrostatics. We will solve the equation under homogeneous boundary conditions

$$(2.2) \quad u(0) = u(L) = 0$$

although it is straightforward to extend to more complicated problems.

2.1. Self-adjoint form (5 points). Show that the problem defined above is self-adjoint.

2.2. Eigenfunctions (5 points). Instead of solving the inhomogeneous problem in Eq. 2.1, solve the related eigenvalue problem

$$(2.3) \quad -\nabla \cdot (\epsilon(x)\nabla\phi_\lambda(x)) + \kappa^2(x)\phi_\lambda(x) = \lambda\phi_\lambda(x)$$

using the same boundary conditions (Eq. 2.2) and assuming $\epsilon(x) = \epsilon$ and $\kappa^2(x) = \kappa^2$ are constant. Use the boundary conditions to specify specific allowable values for λ .

2.3. Using an eigenfunction basis (5 points). As we saw in the linear algebra lectures, eigenfunctions (eigenvectors) provide a very easy basis for solving linear problems. Rewrite Eq. 2.1 using a solution based on a linear combination of eigenfunctions

$$(2.4) \quad u(x) = \sum_{\lambda} \alpha_{\lambda} \phi_{\lambda}(x).$$

Use the orthogonality of the $\{\phi_{\lambda}(x)\}$ to solve the problem for $u(x)$ by deriving an expression for the linear expansion coefficients $\{\alpha_{\lambda}\}$.

2.4. Green function (5 points). The Green function is the solution to a problem with a Dirac delta function source term. In the context of the current problem, the Green function is the potential due to a point charge. Solve Eq. 2.1 for $\rho(x) = \delta(x - x_0)$ where $x_0 \in [0, L]$ to determine the Green function for this problem. Use the property of the delta function

$$(2.5) \quad \int_0^L f(x)\delta(x - x_0)dx = f(x_0)$$

to simplify your answer. Assume $L = 1$ and $x_0 = 1/2$ and plot your solution (in Matlab or Mathematica) for various values of ϵ and κ^2 .

3. RECOVERY FROM STRONG PHOTBLEACHING (20 POINTS)

We're going to model the diffusion of fluorophores into a depleted region generated by photobleaching. We'll be modeling this process in the cylindrical domain $0 \leq r \leq b$; e.g., a portion of a membrane. We'll start with an initial concentration profile of

$$(3.1) \quad u(r, 0) = u_0(r) = \begin{cases} 0 & 0 \leq r < a \\ \bar{u} & a < r < b \end{cases}$$

and assume that the system evolves in time according to

$$(3.2) \quad \partial_t u(r, t) = D\nabla^2 u(r, t).$$

This model is appropriate for a "FRAP"-like study (fluorescence recovery after photobleaching) where the initial concentration profile is prepared by high-intensity, long duration photobleaching. Weaker initial photobleaching would create smoother initial distributions.

The system is constant along the cylinder axis (z) and radially-symmetric. We assume that

$$(3.3) \quad u(b, t) = \bar{u}$$

and $0 \leq u(r, t) < \infty$. Solve this problem for $u(r, t)$. Don't worry about plotting your answer unless you're interested in what it looks like – it's not trivial with Matlab but fairly easy with Mathematica. **HINT:** You might want to use the relation

$$(3.4) \quad \int_0^R J_n(r) r dr = R J_1(R)$$

4. NORMAL MODE ANALYSIS (20 POINTS)

We now have all the tools we need to revisit the concept of normal mode analysis, introduced in an *ad hoc* way in the linear algebra lectures. In what follows, we're going to model a linear chain of N oscillators which undergo transverse displacements x_i . We assume the energy of the system is governed by the Hamiltonian

$$(4.1) \quad H(\{x_i\}) = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N k_{ij} x_i x_j$$

where $k_{ij} = k_{ji} \geq 0$ are the spring constants for the system. We assume the equations of motion for each oscillator have the form

$$(4.2) \quad m_i \ddot{x}_i(t) = F_i(\{x_i\}, t)$$

where $m_i > 0$ is the mass of oscillator i and

$$(4.3) \quad F_i = -\frac{\partial H}{\partial x_i}$$

is the force on oscillator i .

4.1. **Matrix equations (7 points)**. Write the equation of motion above (Eq. 4.2) as a matrix equation of the form

$$(4.4) \quad \ddot{\underline{x}}(t) + \underline{\underline{A}} \underline{x}(t) = 0$$

and transform the problem to a new coordinate system $\underline{y}(t)$ which diagonalizes the equations of motion such that

$$(4.5) \quad \ddot{\underline{y}}(t) + \underline{\underline{\Gamma}} \underline{y}(t) = 0$$

where $\underline{\underline{\Gamma}}$ is a diagonal matrix.

4.2. **Solving the ODEs (7 points)**. Now that you have a diagonal system of equations of the form in Eq. 4.5, you can solve each equation

$$(4.6) \quad \ddot{y}_i(t) + \Gamma_{ii} y_i(t) = 0$$

independently. Solve for $\underline{y}(t)$ assuming that $\underline{z}(0) = \underline{x}_0$ and $\underline{\dot{x}}(0) = \underline{v}_0$. Transform the problem back to the original coordinate system to write an expression for $\underline{x}(t)$.

4.3. **Numerical solution (6 points)**. Implement your solution in Matlab for

$$(4.7) \quad k_{ij} = \begin{cases} k_1 & i = j - 1 \\ k_0 & i = j \\ k_1 & i = j + 1 \\ 0 & \text{otherwise} \end{cases}$$

for $k_0 = 2k_1$, m_i , $N > 10$, \underline{x}_0 , and \underline{v}_0 of your choice. What happens as you introduce non-uniformity in the mass?

5. POLYMER PHYSICS (20 POINTS)

For a long Gaussian-chain polymer of length n , the probability $G(\underline{r}, \underline{r}', n)$ of observing one end of the polymer at \underline{r} and another end of the polymer at \underline{r}_0 is given by the differential equation

$$(5.1) \quad \partial_n g(\underline{r}, \underline{r}_0, n) = \frac{b^2}{6} \nabla^2 g(\underline{r}, \underline{r}_0, n)$$

where b is an effective bond length for segments of the polymer chain. We are interested in solving this equation for $n > 0$ in a rectangular box $0 \leq x \leq L_x$, $0 \leq y \leq L_y$, $0 \leq z \leq L_z$ subject to the conditions that chains of zero length have the same start and end points

$$(5.2) \quad g(\underline{r}, \underline{r}_0, 0) = \delta(\underline{r} - \underline{r}_0) = \delta(x - x_0) \delta(y - y_0) \delta(z - z_0)$$

and that the polymer is confined to the inside of the box $\Omega = [0, L_x] \times [0, L_y] \times [0, L_z]$ such that, for $\underline{r}_0 \in \Omega$,

$$(5.3) \quad g(\underline{r}, \underline{r}_0, n) = 0 \text{ for } \underline{r} \in \partial\Omega$$

where $\partial\Omega$ is the boundary of the box. Let's study this polymer!

5.1. The separated problem (5 points). This problem is already homogeneous. Please separate it into ODEs for the functions $X(x)$, $Y(y)$, $Z(z)$, and $N(n)$ such that $g = XYZN$.

5.2. General solution (5 points). Solve your separated equations (and separation constants) subject to the boundary conditions in Eq. 5.3 and, following our usual protocol, write a general solution as a linear combination of your separated solutions.

5.3. **Specific solution (5 points).** Use the condition in Eq. 5.2 to specify the coefficients of linear combination solution from the previous step and thus arrive at the specific solution to this problem.

5.4. **Analyzing the probability (5 points).** Feel free to answer the following questions with any values of \underline{r}_0 , b , L_x , L_y , and L_z you choose. I recommend that $\underline{r}_0 \neq \underline{0}$ and that $b \ll L_x, L_y, L_z$.

- (a) Generate a plot to show how the probability of finding two ends of the chain at the same point $g(\underline{r}, \underline{r}, n)$ changes with chain length n ?
- (b) Generate a plot showing the probability $g(\underline{r}, \underline{r}_0, n)$ on an xy slice through the domain for parameters of your choosing. Where is the end of the chain likely to be?
- (c) What happens to the probability distribution as b gets large with respect to L_x, L_y, L_z ?