18.303 Problem Set 3 Solutions

Problem 1: (5+5+10+10+5)

(a) $\frac{d}{dt}u_m\Delta x$ is the net rate at which mass diffuses into piece m minuse the rate at which it dissociates:

$$\frac{du_m}{dt}\Delta x = D\frac{u_{m+1}-u_m}{\Delta x} + D\frac{u_{m-1}-u_m}{\Delta x} - Ru_m\Delta x$$

which can be rearranged into

$$\frac{du_m}{dt} = D\frac{u_{m+1}-2u_m+u_{m-1}}{\Delta x^2} - Ru_m.$$

In the $\Delta x \to 0$ limit, the first term is exactly the second derivative, from class, while the second term doesn't change, so we obtain the following PDE for $u(x,t)$:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - Ru$$

(b) This corresponds to $u_0 = u_{M+1} = 0$, or Dirichlet boundary conditions $u(0) = u(L) = 0$.

(c) If there is no flow through the ends, this corresponds to setting

$$D\frac{u_{M+1}-u_M}{\Delta x} = 0 = D\frac{u_0-u_1}{\Delta x},$$

or equivalently $u_{M+1} = u_M$ and $u_0 = u_1$. This makes the u_1 and u_M equations

$$\frac{du_1}{dt} = D\frac{u_2-2u_1+u_1}{\Delta x^2} - Ru_1,$$

$$\frac{du_M}{dt} = D\frac{u_M-2u_M+u_{M-1}}{\Delta x^2} - Ru_M.$$

If we write this in matrix form $d\mathbf{u}/dt = A\mathbf{u}$, we get

$$A = \frac{1}{\Delta x^2}\begin{pmatrix} -1 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -1 \end{pmatrix} - RI$$

where I is the identity matrix, and the first matrix is the same as our second-derivative matrix from class except for the first and last rows. In the continuum limit, setting $\frac{u_{m+1}-u_m}{\Delta x} = 0$ corresponds to setting the first derivative to zero at the ends, i.e. we have the (Neumann) boundary conditions $\frac{\partial u}{\partial x} = 0$ at $x = 0, L$.

(d) The operator in both cases is $\hat{A} = \frac{\partial^2}{\partial x^2} - R$. We will use the usual inner product $\langle u, v\rangle = \int_0^L \bar{u}v$. The R term is just a real number and hence is Hermitian ($\langle u, Rv\rangle = \langle Ru, v\rangle$ by inspection). The $\frac{\partial^2}{\partial x^2}$ term was already shown in class to be Hermitian for Dirichlet boundary conditions. For Neumann boundary conditions, we integrate by parts

$$\langle u, v''\rangle = \int_0^L \bar{u}v'' = \bar{u}\cancel{v'}\Big|_0^L - \int_0^L \overline{u'}v' = -\cancel{\bar{u}'}v\Big|_0^L + \int_0^L \overline{u''}v = \langle u'', v\rangle,$$

in which the boundary terms again vanish so we obtain that $\hat{A} = \hat{A}^*$. To show definiteness, as in class we just integrate by parts once, which with either boundary condition gives

$$\langle u, \hat{A}u\rangle = -\int_0^L \left(|u'|^2 + R|u|^2\right)dx \le 0,$$

which is < 0 unless $u = 0$ almost everywhere, due to the R term alone (since $R > 0$ was given). Hence it is negative-definite. If we set $R = 0$, then with Dirichlet boundary conditions it is still negative-definite as proved in class. For $R = 0$ and Neumann boundary conditions, however, $\langle u, \hat{A}u \rangle = 0 \implies u' = 0 \implies u = \text{constant} \cancel{\implies u = 0}$: nonzero constants are allowed by the boundary conditions, so, e.g. $\langle 1, \hat{A}1 \rangle = 0$ is allowed. Hence $\hat{A}$ is negative semidefinite for Neumann boundaries.

When it is negative-definite ($R > 0$ and/or Dirichlet), that means that the solutions decay to zero as $t \to \infty$, as discussed in class (each eigenfunction decays as $e^{\lambda t}$ and $\lambda < 0$). When it is only negative semidefinite ($R = 0$ with Neumann boundary conditions), then the solutions decay to constants (the eigenfunction $u = 1$ with $\lambda = 0$ does not decay, while all of the other eigenfunctions decay exponentially)

(e) In this case we get

$$\frac{du_m}{dt} = \frac{D_{m+0.5}\frac{u_{m+1}-u_m}{\Delta x} + D_{m-0.5}\frac{u_{m-1}-u_m}{\Delta x}}{\Delta x} - R_m u_m$$

which goes to the the PDE

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right) - Ru.$$

That is, our difference equation is a finite-difference approximation to taking the derivative, then multiplying by $D(x)$, then taking another deriavive.

As shown in class, the operator on the right-hand-side is still Hermitian and negative definite (or semidefinite if $R = 0$ and we have Neumann boundaries), so the qualitative behavior of the PDE does not change.