Solutions to Homework Set 5

1) Linear Differential operators:

a) Integrating by parts gives us

$$\begin{aligned}\langle u|Lv\rangle_w &= \int_a^b wu^*\left(i\frac{d}{dx}v\right)dx\\ &= [iwu^*v]_a^b + \int_a^b w\left(\frac{i}{w}\frac{d}{dx}wu\right)^* v\,dx\\ &\equiv \quad [Q]_a^b \quad + \quad \langle L^\dagger u|v\rangle_w.\end{aligned}$$

Therefore the formal adjoint is

$$L^\dagger = \frac{i}{w}\frac{d}{dx}w \equiv i\frac{d}{dx} + i(\ln w)',$$

and the boundary term is

$$Q[u,v] = iwu^*v.$$

b) We have that

$$\frac{d}{dx}[u^*v^{(3)} - (u')^*v'' + (u'')^*v' - (u^{(3)})^*v] = u^*v^{(4)} - (u^{(4)})^*v$$

and so

$$\int_0^1 u^*v^{(4)}\,dx = [u^*v^{(3)} - (u')^*v'' + (u'')^*v' - (u^{3)})^*v]_0^1 + \int_0^1 (u^{(4)})^*v\,dx.$$

The formal adjoint $M^\dagger$ is therefore d^4/dx^4, which is the same as M. The operator is therefore *formally* self-adjoint. Is it *truly* self-adjoint? We are told that $\mathcal{D}(M)$ is defined by requiring v and $v^{(3)}$ to be zero at both ends, but we are told nothing about v'' and v'. To make the integrated-out term vanish we therefore need to impose $u'=0$ and $u''=0$ at $x=0,1$. Thus

$$\mathcal{D}(M^\dagger) = \{u, u^{(4)} \in L^2[0,1] \,:\, u'(0)=u'(1)=u''(0)=u''(1)=0\}.$$

These are not the same boundary conditions as those imposed on M, and so M is not truly self-adjoint.

2) Sturm-Liouville forms: The equation $p_0y'' + p_1y' + p_2y = 0$ becomes

$$Ly = \frac{1}{w}(wp_0y')' + p_2y = 0,$$

provided we take

$$w(x) = \frac{1}{p_0}\exp\left\{\int^x \left(\frac{p_1(\xi)}{p_0(\xi)}\right)d\xi\right\}.$$

a) We apply the general method, and so compute

$$\int^x \left(\frac{p_1}{p_2}\right) d\xi = \int^x \left\{\frac{\mu-\nu}{1-\xi^2} - (\mu+\nu+2)\frac{\xi}{1-\xi^2}\right\} d\xi = \ln[(1+x)^{\mu+1}(1-x)^{\nu+1}].$$

Therefore $w = (1+x)^\mu(1-x)^\nu$, and

$$Ly = (1+x)^{-\mu}(1-x)^{-\nu}\frac{d}{dx}\left((1+x)^{\mu+1}(1-x)^{\nu+1}\frac{dy}{dx}\right).$$

When n is an integer, the equation

$$\frac{d}{dx}\left((1+x)^{\mu+1}(1-x)^{\nu+1}\frac{dy}{dx}\right) + n(n+\mu+\nu+1)(1+x)^\mu(1-x)^\nu y = 0$$

has polynomial solutions $y = P_n^{(\nu,\mu)}(x)$. These are the *Jacobi* polynomials.

b) Just set $\mu = \nu = 1/2$.

c) We find $w = 1 - x^2$, and

$$Lu = (1-x^2)^{-1}\frac{d}{dx}\left((1-x^2)\frac{du}{dx}\right) - \frac{m^2}{1-x^2}u.$$

This is the differential operator appearing in *Legendre's equation*.

3) Discrete approximations and self-adjointness: Matrices whose only non-zero entries lie on the main diagonal and the diagonals immediately above and below it are called *Jacobi matrices*. Jacobi matrix equations are related to three term recurrence relations of the form

$$au_{n+1} + bu_n + cu_{n-1} = g_n,$$

where the coefficients a, b, and c may depend on n. Such three-term recurrence relations are the natural analogues of second order differential equations because they have a two-dimensional vector space of solutions. These are specified by choosing values for u_0 and u_1, from which all other u_n may then be found by repeated use of the recurrence relation. This is just like the differential equation where we are free to select $y(0)$ and $y'(0)$, but the equation determines all other $y(x)$. In Jacobi matrix problems, the u_n are then restricted by the boundary conditions implicit in the modification of the recurrence relation at the top and bottom row of the matrix.

a) For Dirichlet boundary contitions the boundary values u_0 and u_N are both to zero. We do not bother to store them in memory, and so equation the computer solves will be

$$\begin{pmatrix} g_{N-1} \\ g_{N-2} \\ g_{N-3} \\ \vdots \\ g_3 \\ g_2 \\ g_1 \end{pmatrix} = \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & 1 & -2 & 1 & 0 \\ 0 & \dots & 0 & 0 & 1 & -2 & 1 \\ 0 & \dots & 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_{N-1} \\ u_{N-2} \\ u_{N-3} \\ \vdots \\ u_3 \\ u_2 \\ u_1 \end{pmatrix}.$$

The matrix is real symmetric.

b) For periodic boundary conditions, we imagine additional sites u_0 and u_{N+1} beyond the range of stored variables, and wrap the column vector by setting $u_0 = u_N$ and $u_{N+1} = u_1$. The computer therefore solves

$$\begin{pmatrix} g_N \\ g_{N-1} \\ g_{N-2} \\ \vdots \\ g_3 \\ g_2 \\ g_1 \end{pmatrix} = \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & \dots & 1 \\ 1 & -2 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & 1 & -2 & 1 & 0 \\ 0 & \dots & 0 & 0 & 1 & -2 & 1 \\ 1 & \dots & 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_N \\ u_{N-1} \\ u_{N-2} \\ \vdots \\ u_3 \\ u_2 \\ u_1 \end{pmatrix}.$$

Despite the 1's in the bottom left and top right corners, the new matrix is still real and symmetric.

c) i) The null space is spanned by solutions of

$$u_{n+1} - 2u_n + u_{n-1} = 0.$$

We do not having to worry about what values to assign to u_0 and u_{N+1}, because the 0's in the top and bottom rows of the matrix suppress their contributions. This is the discrete analogue of a second-order ODE with *no* boundary conditions. Since the recurrence relation has constant coefficients, we try $u_n = \alpha^n$ and find that this is a solution, provided that

$$\alpha^2 - 2\alpha + 1 = (\alpha - 1)^2 = 0.$$

The two roots of this equation coincide. We have therefore found only one of the two linearly independent solutions, *viz*: $u_n = 1^n \equiv 1$. When two roots α and β become degenerate we can find the second solution by taking a suitable linear combination of α^n and β^n that remains finite and linearly independent as $\beta \to \alpha$:

$$\lim_{\beta \to \alpha} \left(\alpha \frac{\alpha^n - \beta^n}{\alpha - \beta} \right) = n\alpha^n$$

The second solution is therefore $u_n = n1^n = n$, as is easily verified. The general null-space element is therefore

$$u_n = a + bn.$$

ii) These discrete null-space vectors correspond to the continuum functions $u(x) = a + bx$, which span the null-space of d^2/dx^2, again with with *no* boundary conditions.

iii) The transposed matrix acts on the column vector in a manner that is indifferent to the stored values of u_1 and u_N. The computer program is therefore effectively setting u_1 and u_N to zero. We have already set to zero, but not bothered to store, u_0 and u_{N+1}. Thus the boundary value and the slope of the continuum $u(x)$ have been set to zero at both end of the interval. The continuum boundary conditions are therefore $u(0) = u'(0) = 0$, $u(1) = u'(1) = 0$. These are indeed the continuum adjoint boundary conditions for $L = d^2/dx^2$ with no boundary conditions.

4) Factorization: This technology is now called *supersymmetric quantum mechanics*, but despite this modern sounding name, the factorization method goes back to Schrödinger in the 1930's.

a) We plug $\psi = \exp\{-\int^x u(\xi)\,d\xi\}$ into the given eqution, and from

$$\frac{d^2\psi}{dx^2} = (u^2 - u')\psi,$$

we find that $W(x) = u^2(x) - u'(x)$. Now

$$M^\dagger M = \left(-\frac{d}{dx} + u(x)\right)\left(\frac{d}{dx} + u(x)\right) = -\frac{d^2}{dx^2} + u^2(x) - u'(x),$$

and so $L = M^\dagger M$.

b) Let ψ_- be an eigenfunction of $M^\dagger M$ with eigenvalue λ. By the associativity of the operator product, we have

$$\lambda M\psi_- = M(M^\dagger M\psi_-) = MM^\dagger(M\psi_-)$$

and so $\psi_+ \equiv M\psi_-$ is an eigenfunction of

$$MM^\dagger = \left(\frac{d}{dx} + u(x)\right)\left(-\frac{d}{dx} + u(x)\right) = -\frac{d^2}{dx^2} + u^2(x) + u'(x),$$

with the same eigenvalue. Similarly, given an eigenfunction ψ_+ of $MM^\dagger$, the function $\psi_- \equiv M^\dagger\psi_-$ is an eigenfunction of $M^\dagger M$ with the same eigenvalue. This pairing of eigenfunctions will fail if and only if $M\psi_- = 0$. If this is the case, then it is obvious that $M^\dagger M\psi_- = 0$, and so $\lambda = 0$. Conversely, suppose that λ is zero, and hence $M^\dagger M\psi_- = 0$. Then

$$0 = \langle\psi_-|M^\dagger M\psi_-\rangle = \langle M\psi_-|M\psi_-\rangle, \quad \Rightarrow M\psi_- = 0.$$

The correspondence $\psi_- \leftrightarrow \psi_+$ therefore fails if, and only if, the eigenvalue is zero. For all other eigenvalues the spectrum of $M^\dagger M$ and $MM^\dagger$ coincide. The pair of Schrödinger operators $L_+ = MM^\dagger$ and $L_- = M^\dagger M$, containing the potentials

$$W_\pm = u^2 \pm u',$$

are said to constitute a *supersymmetric pair*.

c) For $u = \tanh x$ we have

$$\begin{aligned} W_-(x) = u^2 - u' &= \tanh^2 x - \text{sech}^2 x = 1 - 2\text{sech}^2 x, \\ W_+(x) = u^2 + u' &= \tanh^2 x + \text{sech}^2 x = 1, \end{aligned}$$

and so the operators

$$\begin{aligned} L_- &= -\frac{d^2}{dx^2} + 1 - 2\text{sech}^2 x, \\ L_+ &= -\frac{d^2}{dx^2} + 1, \end{aligned}$$

have paired eigenvalues, with the exception of any zero modes. The eigenvalues and eigenfunctions of L_+ are easy to find. The eigenfunctions are

$$\psi_k(x) = e^{ikx}, \quad k \in \mathbb{R}$$

and the corresponding eigenvalues are $\lambda = k^2 + 1$. There is no $\lambda = 0$ zero mode. We now use the results of parts a) and b) to deduce that

$$\begin{aligned} \chi_k(x) &= M^\dagger \psi_k = \left(-\frac{d}{dx} + \tanh x\right) e^{ikx} \\ &= (-ik + \tanh x) e^{ikx} \end{aligned}$$

are eigenfunctions of L_- with eigenvalues $\lambda = k^2 + 1$, and hence eigenfunctions of H with $E = k^2$.

We also know that that if $L_- = M^\dagger M$ is to have a zero mode, then the corresponding eigenfunction will obey the *first order* ODE $M\psi_0 = 0$. Thus we seek a solution to

$$\left(\frac{d}{dx} + \tanh x\right) \psi_0 = 0.$$

This is easy to solve, and we find

$$\begin{aligned} \psi_0(x) &= \exp\left\{-\int^x \tanh \xi \, d\xi\right\} \\ &= \exp\{\ln \operatorname{sech} x\} \\ &= \operatorname{sech} x. \end{aligned}$$

This is a normalizable function, and hence an element of $L^2[\mathbb{R}]$, because

$$\|\psi_0\|^2 = \int_{-\infty}^{\infty} \operatorname{sech}^2 x \, dx = [\tanh x]_{-\infty}^{\infty} = 2.$$

It is a bound-state eigenfunction of H with eigenvalue $E = -1$.

If we try to use this method to find the non-existent zero mode for L_+, we see that it the putative zero-mode eigenfunction would have to obey

$$M^\dagger \psi_0 = \left(-\frac{d}{dx} + \tanh x\right) \psi_0 = 0,$$

and therefore

$$\begin{aligned} \psi_0(x) &= \exp\left\{\int^x \tanh \xi \, d\xi\right\} \\ &= \exp\{-\ln \operatorname{sech} x\} \\ &= \cosh x. \end{aligned}$$

This function does indeed satisfy $L_+\psi_0 = 0$, but it is not normalizable, so not an element of $L^2[\mathbb{R}]$, and therefore not an eigenfunction.