SOLUTIONS TO TEST 2

SEPARATION OF VARIABLES (estimated time $\sim$ 20 min):

1) Consider the two-dimensional Schrödinger equation

$$-\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right)=E\psi, \qquad x\in[0,a], \quad y\in[0,b], \tag{1}$$

where $\psi=\psi(x,y)$ is a wavefunction, E is the energy, and a and b are the dimensions of the rectangle spanned by x and y. The wavefunction must satisfy the boundary conditions

$$\frac{\partial\psi(0,y)}{\partial x}=\frac{\partial\psi(a,y)}{\partial x}=0, \qquad \psi(x,0)=\psi(x,b)=0, \tag{2}$$

which imposes constraints on the separation constant and the energy E, for a non-trivial wavefunction to exist, i.e., a wavefunction which is not identically zero. Write $\psi(x,y)=F(x)G(y)$ and use separation of variables to determine the smallest energy $E_{\min}$, for which a non-trivial wavefunction can exist.

SOLUTION:

1.1) We insert the assumption $\psi(x,y)=F(x)G(y)$ into Eq. (1) and obtain the equation

$$-F_{xx}G-FG_{yy}=EFG \quad\Rightarrow\quad -\frac{F_{xx}}{F}=\frac{G_{yy}}{G}+E,$$

where subscript denotes differentiation. In the last equation the left hand side depends only on x, while the right hand side depends only on y. This can only be satisfied if both sides are equal to the same constant λ. Because we have homogeneous boundary conditions we can then separate into the following two equations

$$\begin{aligned} F_{xx}&=-\lambda F, &\qquad F_x(0)&=F_x(a)=0,\\ G_{yy}&=(\lambda-E)G, &\qquad G(0)&=G(b)=0. \end{aligned}$$

Let us look at the equation for $F(x)$ first: For λ=0 we obtain the solution

$$F_{xx}=0 \quad\Rightarrow\quad F(x)=c_0+d_0x \quad\Rightarrow\quad F_x(0)=F_x(a)=d_0=0 \quad\Rightarrow\quad F(x)=c_0.$$

Thus λ=0 is an eigenvalue with eigenfunction c_0. For $\lambda=-k^2<0$ we obtain the solution

$$F(x)=c_1\mathrm{e}^{kx}+d_1\mathrm{e}^{-kx}.$$

The left boundary condition is $F_x(0)=k(c_1-d_1)=0$. Thus $F(x)=2c_1\cosh(kx)$ and the right boundary condition $F_x(a)=2c_1k\sinh(ka)=0$ cannot be fulfilled unless a=0 (unphysical box) or $c_1=d_1=0$ (trivial zero-solution). Therefore $\lambda<0$ is also not an eigenvalue.

SOLUTIONS TO TEST 2

For $\lambda = k^2 > 0$ *we obtain the solution*

$$F(x) = c_2 \cos(kx) + d_2 sin(kx).$$

The left boundary condition gives

$$F_x(0) = kd_2 = 0 \quad \Rightarrow \quad d_2 = 0 \quad \Rightarrow \quad F(x) = c_2 \cos(kx).$$

To obtain a nontrivial solution we must therefore require that $c_2 \neq 0$ *and again* $a > 0$ *to have a physical box size. The right boundary condition then gives us the eigenvalues*

$$F_x(a) = -kc_2 \sin(ka) = 0 \quad \Rightarrow \quad \lambda = \lambda_n = k_n^2 = \left(\frac{n\pi}{a}\right)^2, \quad n = 1, 2, 3...$$

Now we remember that λ*=0 was an eigenvalue with the eigenfunction being a constant. This case is contained in the above expression, and thus we may combine them and write the final solution*

$$F = F_n(x) = A_n \cos(\sqrt{\lambda_n}\, x), \quad \lambda_n = \left(\frac{n\pi}{a}\right)^2, \quad n = 0, 1, 2, 3...$$

We can now write the equation for $G(y)$ *in the form*

$$G_{yy} = -\gamma G, \qquad G(0) = G(b) = 0 \qquad \gamma = E - \lambda_n.$$

For γ*=0 the solution is* $G(y)$*=*$c_3 + d_3 y$ *and the boundary conditions* $G(0)$*=*c_3*=0 and* $G(b)$*=*$d_3 b$*=0 can only be fulfilled by the trivial zero-solution* c_3*=*d_3*=0 or an unphysical box size b=0. Thus* γ*=0 is not an eigenvalue.*

For γ*=*$-\kappa^2$*<0 the solution is* $G(y)$*=*$c_4 \exp(\kappa y) + d_4 \exp(-\kappa y)$*. The boundary condition* $G(0)$*=*$c_4 + d_4$*=0 gives* $G(y)$*=*$2c_4 \sinh(\kappa y)$ *and therefore* $G(b) = 2c_4 \sinh(\kappa b) = 0$ *can only be fulfilled by the trivial zero-solution* c_4*=*d_4*=0 or an unphysical box size b=0. Thus* $\gamma < 0$ *is also not an eigenvalue.*

Finally, for $\gamma = \kappa^2 > 0$ *we obtain the solution* $G(y) = c_5 \cos(\kappa y) + d_5 sin(\kappa y)$*. The left boundary condition gives* $G(0)$*=*c_5*=0 and thus* $G(y)$*=*$d_5 \sin(\kappa y)$*. To obtain a nontrivial solution we must therefore require that* $d_5 \neq 0$ *and* $b > 0$ *to have a physical box size. The right boundary condition then gives us the eigenvalues*

$$G(b) = d_5 \sin(\kappa b) = 0 \quad \Rightarrow \quad \gamma = \gamma_m = \kappa_m^2 = \left(\frac{m\pi}{b}\right)^2, \quad m = 1, 2, 3...$$

We can now determine the minimum energy from the relation E*=*$\gamma_m + \lambda_n$ *as follows*

$$E = \gamma_m + \lambda_n = \left(\frac{m\pi}{b}\right)^2 + \left(\frac{n\pi}{a}\right)^2 \geq \left(\frac{\pi}{b}\right)^2 = E_{\min},$$

because $n \geq 0$ *and* $m \geq 1$*. Note how it was not necessary to write up the full solution to find the minimum energy.*

SOLUTIONS TO TEST 2

GREEN'S FUNCTION (estimated time $\sim$ 15 min.):

2) Consider the following equation

$$\frac{d^2u}{dx^2} = f(x), \qquad x \in [0,1], \qquad u(0) = u(1) = 0, \tag{3}$$

for the function u=$u(x)$. Find Green's function $G(x, x')$ for the problem (3).

SOLUTION:

2.1) First we note that the boundary conditions are homogeneous and thus we may apply Green's function approach directly with the same homogeneous boundary conditions. We define Green's function $G(x, x')$ to be a solution to the problem

$$\frac{d^2G}{dx^2} = \delta(x - x'), \qquad G(0, x') = G(1, x') = 0, \qquad x \in [0,1], \qquad x' \in]0,1[\tag{4}$$

For $0 \leq x < x'$ Green's function satisfies the homogeneous equation d^2G/dx^2=0 and we obtain the solution

$$G = G_1(x, x') = Ax + B \quad \Rightarrow \quad G_1(0, x') = B = 0 \quad \Rightarrow \quad G_1(x, x') = Ax.$$

For $x' < x \leq 1$ Green's function satisfies also the homogeneous equation d^2G/dx^2=0 and we obtain the solution

$$G = G_2(x, x') = C(x-1) + D \quad \Rightarrow \quad G_2(1, x') = D = 0 \quad \Rightarrow \quad G_2(x, x') = C(x-1).$$

Integrating Eq. (4) from $x' - \epsilon$ to $x' + \epsilon$ and letting $\epsilon \to 0$ we obtain the condition

$$\left.\frac{dG_2}{dx}\right|_{x=x'} - \left.\frac{dG_1}{dx}\right|_{x=x'} = C - A = 1 \quad \Rightarrow \quad C = A + 1.$$

From Eq. (4) we see that d^2G/dx^2 has a δ-function in x' and that dG/dx has a discontinuity in x'. This means that Green's function itself is continuous in x', which gives the requirement

$$G_2(x', x') = G_1(x', x') \quad \Rightarrow \quad Ax' = C(x'-1) = (A+1)(x'-1) \quad \Rightarrow \quad A = x' - 1.$$

The expression for Green's function is therefore

$$G(x, x') = \begin{cases} (x'-1)x & \text{for} \quad 0 \leq x < x' \\ (x-1)x' & \text{for} \quad x' < x \leq 1 \end{cases}$$

As a check we note that Green's function $G(x, x')$ is symmetric in its arguments, as it should be. We know that this should be the case because the operator $\hat{L} = d^2/dx^2$ appearing in Eq. (3) is a Sturm-Liouville operator and Green's function is reel.