M.Sc. Course No. 02647, Fall 2002
Applied Mathematics for Physicists

# *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 $\lambda$. Because we have homogeneous boundary conditions we can then separate into the following two equations*

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

*Let us look at the equation for $F(x)$ first: For $\lambda$=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 $\lambda$=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.*

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*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 $\lambda$=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 $\gamma$=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 $\gamma$=0 is not an eigenvalue.*

*For $\gamma$=$-\kappa^2$<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*

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

*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 ~ 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* $0 \le x < x'$ *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* $x' < x \le 1$ *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* $\delta$*-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*

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

*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.*