School of Mathematical Sciences

THE UNIVERSITY OF ADELAIDE AUSTRALIA

Assessment Cover Sheet

Student Name	Andrew Martin
Student ID	1704466
Assignment Number	5
Course	
Tutorial Group	

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PDEs and Waves, Assignment 5

Andrew Martin

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1. Previous assignment question mark is 1/5

2. Consider, in any dimension, the following eigenproblem for $v(\vec{x})$ and λ:

$$\nabla \cdot (p(\vec{x})\nabla v) + q(\vec{x})v + \lambda r(\vec{x})v = 0 \quad \text{in domain } D,$$

with real coefficient functions where $p(\vec{x}), r(\vec{x}) > 0$ in D, and with boundary conditions on ∂D of (set $\alpha_2 = 1$ for a little simplicity)

$$\alpha_1 v + \frac{\partial v}{\partial n} = 0\,, \quad \text{where } n \text{ is the normal direction.}$$

Use Green's formula to prove that there cannot be any generalised eigenfunctions: recall that such generalised eigenfunctions w are defined as satisfying both $\mathcal{L}w + \lambda r w = rv$ and the same boundary conditions. Use contradiction.

Solution Greens formula:

$$\int_a^b v\mathcal{L}w - w\mathcal{L}v d\vec{x} = \int_{\partial D} p\left(v\frac{\partial w}{\partial n} - \frac{\partial v}{\partial n}\right) dA$$

Assume there can be generalised eigenfunctions, w, satisfying $\mathcal{L}w + \lambda r w = rv$ and $\alpha_1 w + \frac{\partial w}{\partial n} = 0$ This means Green's formula must be satisfied for w:

$$\int_a^b v\mathcal{L}w - w\mathcal{L}v d\vec{x} = \int_{\partial D} p\left(v\frac{\partial w}{\partial n} - w\frac{\partial v}{\partial n}\right) dA$$

$$\int_a^b v(rv - \lambda rw) - w\mathcal{L}v d\vec{x} = \int_{\partial D} p\left(v\frac{\partial w}{\partial n} - w\frac{\partial v}{\partial n}\right) dA$$

$$\int_a^b (rv^2 - \lambda vrw) - w\mathcal{L}v d\vec{x} = \int_{\partial D} p\left(v\frac{\partial w}{\partial n} - w\frac{\partial v}{\partial n} + a_1vw - a_1vw\right) dA$$

$$\int_a^b (rv^2 - \lambda vrw) - w\mathcal{L}v d\vec{x} = \int_{\partial D} p\left(v(-a_1w) - w(-a_1v)\right) dA$$

$$\int_a^b (rv^2 - \lambda vrw) - w\mathcal{L}v d\vec{x} = \int_{\partial D} p\left(-a_1vw + a_1vw\right) dA$$

$$\int_a^b (rv^2 - \lambda vrw) - w(rw - \lambda rv) d\vec{x} = \int_{\partial D} 0 dA$$

$$\int_a^b rv^2 - rw^2 d\vec{x} = 0$$

Contradiction as r and v are both non-zero.
i.e. there cannot be generalised eigenfunctions w

3. From quantum mechanics, we are given the complex-valued quantum wavefunction field $\psi(\vec{x}, t)$ for a quantum 'particle' satisfies the (nondimensional) Schrodinger PDE

$$-i\frac{\partial \psi}{\partial t} = \nabla^2\psi - V(\vec{x})\psi$$

for $i = \sqrt{-1}$, some fixed (real valued) potential $V(\vec{x})$, and Laplacian ∇^2. Here consider the PDE on the domain D of all 3D space, assuming the boundary condition that $\psi \to 0$ (sufficiently quickly) as $|\vec{x}| \to \infty$.

(a) Use separation of variables, $\psi = v(\vec{x})T(t)$, to derive an ODE for the time evolution, and also a self-adjoint PDE eigenproblem for the spatial structure.

Solution

$$\psi_t = v(\vec{x})\ddot{T}(t)$$

$$\nabla^2\psi = \nabla^2(v(\vec{x})T(t)) = T(t)\nabla^2 v(\vec{x})$$

$$
\begin{aligned}
-i\frac{\partial\psi}{\partial t} &= \nabla^2\psi - V(\vec{x})\psi \\
\implies -iv(\vec{x})\ddot{T}(t) &= T(t)\nabla^2 v(\vec{x}) - V(\vec{x})v(\vec{x})T(t) \\
-i\frac{\ddot{T}(t)}{T(t)} &= \frac{\nabla^2 v(\vec{x}) - V(\vec{x})v(\vec{x})}{v(\vec{x})} = -\lambda
\end{aligned}
$$

Which gives the ODE for time:

$$
-i\frac{\ddot{T}(t)}{T(t)} = -\lambda
$$

And the PDE for space:

$$
\begin{aligned}
\nabla^2 v(\vec{x}) - V(\vec{x})v(\vec{x}) &= -\lambda v(\vec{x}) \\
\nabla^2 v(\vec{x}) - V(\vec{x})v(\vec{x}) + \lambda v(\vec{x}) &= 0
\end{aligned}
$$

This is self-adjoint as it is in form

$$
\nabla p(\nabla v) + qv + \lambda rv = 0
$$

(In this case: $p = 1 \quad q = -V(\vec{x}) \quad r = 1$)

(b) Describe in a paragraph what the multi-dimensional Sturm–Liouville theory then tells us about the modes of the Schrodinger PDE.

Solution The problem must have real (positive) eigenvalues, and hence real frequencies;
with an infinite number of modes of oscillation of indefinitely high frequency;
the spatial patterns of oscillation of the quantum 'particle' are orthogonal.

(c) Write down the Rayleigh quotient. Use it to derive that in the case of radially symmetric potentials in 3D, $V(\vec{x}) = V(r)$ for radius $r = |\vec{x}|$, any radially symmetric eigenfunctions $v(\vec{x}) = v(r)$ have corresponding eigenvalue

$$
\lambda = \frac{\int_0^\infty \left[(dv/dr)^2 + V(r)v^2 \right] r^2\,dr}{\int_0^\infty v^2 r^2\,dr}\,.
$$

Solution Given the form from the previous question, the Rayleigh quotient has form

$$
\begin{aligned}
\lambda &= \frac{-\int_{\partial D} pv\frac{\partial v}{\partial n}dA + \int_D p|\nabla v|^2 - qv^2 d\vec{x}}{\int_D v^2 r(x)dx} \\
&= \frac{-\int_{\partial D} 0dA + \int_D |\nabla v(r)|^2 + V(\vec{x})v(\vec{x})^2 d\vec{x}}{\int_D v(\vec{x})^2 dx} \\
&= \frac{0 + \int_D |dv/dr|^2 + V(\vec{x})v(\vec{x})^2 d\vec{x}}{\int_D v(\vec{x})^2 dx} \\
&= \frac{\int_0^\infty (dv/d\vec{x})^2 + V(r)v(r)^2 d\vec{x}}{\int_0^\infty v(\vec{x})^2 dx} \\
\lambda &= \frac{\int_0^\infty \left[(dv/dr)^2 + V(r)v^2\right] r^2\, dr}{\int_0^\infty v^2 r^2\, dr}
\end{aligned}
$$

(d) Use the Rayleigh quotient to estimate the smallest eigenvalue (the lowest energy state for a quantum particle) in a parabolic potential well $V(\vec{x}) = |\vec{x}|^2 = r^2$ in 3D. Make the rough approximation that the lowest eigenvalue corresponds to a single-humped 'parabolic' eigenfunction

$$
v(r) \approx \begin{cases} 1 - r^2/a^2 & r \leq a\,, \\ 0 & r \geq a\,, \end{cases}
$$

for some (real) parameter $a > 0$ to be decided. Decide parameter a by the heuristic of requiring $d\lambda/da = 0$; that is, that the approximate eigenvalue is to be least sensitive to our imposed assumption that the field v is nonzero only for radii $r = |\vec{x}| < a$.

Solution

$$
\begin{aligned}
\lambda &= \frac{\int_0^\infty \left[(dv/dr)^2 + V(r)v^2 \right] r^2\,dr}{\int_0^\infty v^2 r^2\,dr} \\
&= \frac{\int_0^a \left[(dv/dr)^2 + V(r)v^2 \right] r^2\,dr + \int_a^\infty \left[(dv/dr)^2 + V(r)v^2 \right] r^2\,dr}{\int_0^a v^2 r^2\,dr + \int_a^\infty v^2 r^2\,dr} \\
&= \frac{\int_0^a \left[(dv/dr)^2 + V(r)v^2 \right] r^2\,dr + \int_a^\infty 0\,dr}{\int_0^a v^2 r^2\,dr + \int_a^\infty 0\,dr} \\
&= \frac{\int_0^a \left[(dv/dr)^2 + V(r)v^2 \right] r^2\,dr}{\int_0^a v^2 r^2\,dr} \\
&= \frac{\int_0^a \left[\left(d(1-r^2/a^2)/dr\right)^2 + r^2(1-r^2/a^2)^2 \right] r^2\,dr}{\int_0^a (1-r^2/a^2)^2 r^2\,dr} \\
&= \frac{\int_0^a \left[4r^2/a^4 + r^2(1-2r^2/a^2+r^4/a^4) \right] r^2\,dr}{\int_0^a (1-2r^2/a^2+r^4/a^4) r^2\,dr} \\
&= \frac{\int_0^a \left[4r^2/a^4 + r^2 - 2r^4/a^2 + r^6/a^4 \right] r^2\,dr}{\int_0^a r^2 - 2r^4/a^2 + r^6/a^4\,dr} \\
&= \frac{\int_0^a 4r^4/a^4 + r^4 - 2r^6/a^2 + r^8/a^4\,dr}{\int_0^a r^2 - 2r^4/a^2 + r^6/a^4\,dr} \\
&= \frac{r^9/9a^4 + 4r^5/5a^4 - 2r^7/7a^2 + r^5/5|_0^a}{r^7/7a^4 - 2r^5/5a^2 + r^3/3|_0^a} \\
&= \frac{a^9/9a^4 + 4a^5/5a^4 - 2a^7/7a^2 + a^5/5}{a^7/7a^4 - 2a^5/5a^2 + a^3/3} \\
&= \frac{a^5/9 + 4a/5 - 2a^5/7 + a^5/5}{a^3/7 - 2a^3 + a^3/3} \\
\lambda &= -\frac{21((8a^5)/315 + (4a)/5)}{32a^3} \\
d\lambda/da &= 0 \\
\frac{63-2a^4}{60a^3} &= 0 \\
a &= \sqrt{3}\sqrt[4]{7/2} \\
\implies \lambda &= -\sqrt{7/2}/10
\end{aligned}
$$

4. Explore an alternative simple space-time discretisation of the linear 1D wave PDE $u_t + cu_x = 0$. Define time grid points $t_\ell = \ell\tau$ with time step τ, define space grid points $x_j = jh$ with space step h, and define the grid values $u_j^\ell = u(x_j, t_\ell)$.

   (a) Consider the wave PDE $u_t + cu_x = 0$ at the point $(x_j, t_{\ell+1})$: approximate the spatial derivative by a centred difference, and the time derivative using only u_j^ℓ and $u_j^{\ell+1}$. Hence derive the simple discretisation

$$u_j^{\ell+1} + \frac{s}{2}(u_{j+1}^{\ell+1} - u_{j-1}^{\ell+1}) = u_j^\ell,$$

for some particular parameter s.

Solution Using centred difference for x and forward finite difference for t i.e. FTCS.

$$\begin{aligned} \frac{\partial u}{\partial x}\Big|_j^{l+1} &= \frac{u_{j+1}^{l+1} - u_{j-1}^{l+1}}{2h} \\ \frac{\partial u}{\partial t}\Big|_j^{l} &= \frac{u_j^{l+1} - u_j^{l}}{\tau} \end{aligned}$$

Which gives:

$$\begin{aligned} u_t &= -cu_x \\ \frac{u_j^{l+1} - u_j^l}{\tau} &= -c\left(\frac{u_{j+1}^{l+1} - u_{j-1}^{l+1}}{2h}\right) \\ u_j^{l+1} + c\left(\frac{u_{j+1}^{l+1} - u_{j-1}^{l+1}}{2h}\right) &= u_j^l \\ u_j^{l+1} + \frac{s}{2}\left(u_{j+1}^{l+1} - u_{j-1}^{l+1}\right) &= u_j^l \quad s := c\tau/h \end{aligned}$$

(b) Use operator algebra to find the equivalent PDE, including the leading order error, and confirm consistency of this scheme to the original PDE.

Solution Notation: subscripts x and t refer to the operator in regards to x or t,
Write ∂ as differentiation,
ε as a positive grid movement by one step (h or τ),

$$\begin{aligned} u_j^{l+1} + \frac{s}{2}\left(u_{j+1}^{l+1} - u_{j-1}^{l+1}\right) &= u_j^l \\ \varepsilon_t u + \frac{s}{2}(\varepsilon_t\varepsilon_x u - \varepsilon_t\varepsilon_x^{-1}u) &= u \end{aligned}$$

(c) Apply a von Neumann stability analysis to the discretisation to derive the growth factor $G = 1/[1 + is\sin kh\,]$, and hence determine for what range of parameter s there are unstable growing solutions in this scheme: $|G| > 1$, for some wavenumber(s) k.

Solution Subbing in: $u_j^l = G^l e^{ikx} = G^l e^{ikhj}$

$$
\begin{aligned}
u_j^{l+1} + \frac{s}{2}\left(u_{j+1}^{l+1} - u_{j-1}^{l+1}\right) &= u_j^l \\
G^{l+1}e^{ikhj} + \frac{s}{2}\left(G^{l+1}e^{ikh(j+1)} - G^{l+1}e^{ikh(j-1)}\right) &= G^l e^{ikhj} \\
G^{l+1}e^{ikhj} + \frac{s}{2}\left(G^{l+1}e^{ikh(j+1)} - G^{l+1}e^{ikh(j-1)}\right) - G^l e^{ikhj} &= 0 \\
G^l e^{ikhj}\left(G + \frac{s}{2}\left(Ge^{ikh} - Ge^{-ikh}\right) - 1\right) &= 0 \\
G + \frac{s}{2}\left(Ge^{ikh} - Ge^{-ikh}\right) - 1 &= 0 \\
G + G\frac{s}{2}\left(e^{ikh} - e^{-ikh}\right) &= 1 \\
G(1 + \frac{s}{2}\left(e^{ikh} - e^{-ikh}\right)) &= 1 \\
G &= \frac{1}{1 + \frac{s}{2}\left(e^{ikh} - e^{-ikh}\right)}
\end{aligned}
$$

But $e^{ikh} - e^{-ikh} = 2i\sin(kh)$, so:

$$
\begin{aligned}
G &= \frac{1}{1 + \frac{s}{2}\left(e^{ikh} - e^{-ikh}\right)} \\
&= \frac{1}{1 + \frac{s}{2}2i\sin(kh)} \\
\implies G &= \frac{1}{1 + is\sin(kh)}
\end{aligned}
$$

The solutions are unstable if $|G| > 1$

$$
\begin{aligned}
G &= \frac{1}{1 + is\sin(kh)} \\
|G| > 1 \implies &|\frac{1}{1 + is\sin(kh)}| > 1 \\
&1 < |1 + is\sin(kh)| \\
&0 < |s||\sin(kh)| < 2
\end{aligned}
$$

$\sin(kh) \leq 1$ Which gives

$$0 < |s| < 2$$

For $k = \frac{n\pi + \frac{\pi}{2}}{h}$, $n \in Z$

5. The linear Schrodinger PDE not only describes quantum phenomena but also guides the modulation of water waves. Adapt the Crank–Nicolson code for the heat PDE to solve the Schrodinger PDE in one space dimension,

$$-i\psi_t = \psi_{xx} - V(x)\psi\,,$$

for a complex-valued field $\psi(x,t)$ in the domain $|x| \le 4$ over times $0 \le t \le 1$ and with the double well potential $V = (4-x^2)^2$. Use boundary conditions of $\psi = 0$ at $x = \pm 4$, and the initial condition of $\psi(x,0) = \operatorname{sech}[2(x+2.6)]$ corresponding to a particle located to one side of one well.

(a) Following the discretisation of the heat PDE, derive a Crank–Nicolson discretisation of the Schrodinger PDE with differences due to the potential and with a pure imaginary parameter s.

Solution

$$\psi = \frac{\psi_j^l + \psi_j^{l+1}}{2}$$

$$\psi_t|_j^l = \frac{\psi_j^{l+1} - \psi_j^l}{\tau}$$

$$\psi_{xx}|_j^l = \frac{1}{2}\left(\frac{\psi_{j+1}^l - 2\psi_j^l + \psi_{j-1}^l}{h^2} + \frac{\psi_{j+1}^{l+1} - 2\psi_j^{l+1} + \psi_{j-1}^{l+1}}{h^2}\right)$$

So the discretisation will be:

$$-i\psi_t = \psi_{xx} - V(x)\psi$$

$$-i\frac{\psi_j^{l+1} - \psi_j^l}{\tau} = \frac{1}{2}\left(\frac{\psi_{j+1}^l - 2\psi_j^l + \psi_{j-1}^l}{h^2} + \frac{\psi_{j+1}^{l+1} - 2\psi_j^{l+1} + \psi_{j-1}^{l+1}}{h^2}\right) - \frac{1}{2}(4-x^2)^2(\psi_j^l + \psi_j^{l+1})$$

$$\psi_j^{l+1} - \psi_j^l = \frac{-\tau}{2i}\left(\frac{\psi_{j+1}^l - 2\psi_j^l + \psi_{j-1}^l}{h^2} + \frac{\psi_{j+1}^{l+1} - 2\psi_j^{l+1} + \psi_{j-1}^{l+1}}{h^2} - 2\frac{1}{2}(4-x^2)^2(\psi_j^l + \psi_j^{l+1})\right)$$

For $s := \frac{-\tau}{ih^2}$. Rearranging gives:

$$2\psi_j^{l+1} - 2\psi_j^l = s\psi_{j+1}^l - 2s\psi_j^l + s\psi_{j-1}^l + s\psi_{j+1}^{l+1} - 2s\psi_j^{l+1} + s\psi_{j-1}^{l+1} + \frac{\tau}{i}(4-x^2)^2\psi_j^l$$

$$2\psi_j^{l+1} - s\psi_{j+1}^{l+1} + 2s\psi_j^{l+1} - s\psi_{j-1}^{l+1} = 2\psi_j^l + s\psi_{j+1}^l - 2s\psi_j^l + s\psi_{j-1}^l + \frac{\tau}{i}(4-x^2)^2(\psi_j^l + \psi_j^{l+1})$$

So the Solution has form:

$$(2s+2-\frac{\tau}{i}(4-x^2)^2)\psi_j^{l+1} - s\psi_{j+1}^{l+1} - s\psi_{j-1}^{l+1} = s\psi_{j+1}^l + (2-2s)\psi_j^l + s\psi_{j-1}^l + \frac{\tau}{i}(4-x^2)^2\psi_j^l$$

(b) For this part, ignore the potential term: then the discretisation of the linear Schrodinger PDE is equivalent to that for the heat PDE but with imaginary parameter s. In this case, use the expression derived in lectures for the growth factor of the heat PDE to comment on the stability of the discretisation of the linear Schrodinger PDE (when $V = 0$).

Solution So using the discretisation:

$$(2s+2)\psi_j^{l+1} - s\psi_{j+1}^{l+1} - s\psi_{j-1}^{l+1} = s\psi_{j+1}^{l} + (2-2s)\psi_j^{l} + s\psi_{j-1}^{l}$$

Gives the growth factor:

$$G = \frac{1 - s2\sin^2(kh/2)}{1 + s2\sin^2(kh/2)}$$

Since $|G^l|$ decays to zero for all k, this scheme is stable for all s.

(c) Adapt the computer code for the heat PDE to implement the Crank–Nicolson scheme for the linear Schrodinger PDE, debug and execute. Use enough grid points in space and time to obtain a reasonably clean picture of the complicated complex solutions. Visualise the complex field ψ by plotting $|\psi|$ as the height of a surface, and colour the surface with $\arg\psi$ which in Matlab/Octave is computed with `angle()`. Submit your code and plot.

Solution

```
function heatCN
% Compute solutions of heat PDE with Crank−Nicholson
% AJR, 9/9/2014
%Adapted for Schrodinger equation by Andrew Martin
%1704466
%16/10/17
nPoints=61; % number of spatial grid points
x=linspace(−4,4,nPoints)';
j=2:nPoints−1;
h=x(2)−x(1); % space step of grid
nTimes=51; % number of time steps
t=linspace(0,1,nTimes);
tau=t(2)−t(1); % time step
% storage and initial condition
u=nan(nPoints,nTimes);
u(:,1)=sech(2∗(x+2.6));
V = tau/i ∗(4−x(j).^2).^2;
% sparse matrix of the CN scheme
s= i∗tau/h^2;
A=sparse(j,j,2∗(1+s)−V,nPoints,nPoints) ...
```

```
+sparse(j,j-1,-s,nPoints,nPoints) ...
+sparse(j,j+1,-s,nPoints,nPoints) ...
+sparse([1 nPoints],[1 nPoints],1,nPoints,nPoints);
spy(A)
condA=condest(A); % check condition number not large
for l=1:nTimes-1 % time step loop
rhs=[uleft(t(l+1))
s*u(j-1,l)+2*(1-s)*u(j,l)+s*u(j+1,l)+(V.*u(j,l))
uright(t(l+1))];
u(:,l+1)=A\rhs; % solve linear eqns A.u=rhs
end
surf(t,x,abs(u),angle(u))
xlabel('time t'),ylabel('space x'),zlabel('|\psi(x,t)|')
C = colorbar;
C.Label.String = "arg(\psi)";
%-----------------------------------------------------------
function ua=uleft(t), ua=zeros(size(t));
function ub=uright(t), ub=zeros(size(t));
```

Which produces the plot: