**PHYS 440: Do 3 out of 4. PHYS 740: Do 4 out if 4.**

# 1 Thermal Diffusion with Time-Varying Boundary Condition

In this problem, we will consider the fluctuations of the temperature of the Earth's crust with time due to daily and seasonal oscillations. The thermal diffusion equation is:

first derivative wrt time —> Crank-Nicolson

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial z^2}, \tag{1}$$

where $T(z,t)$ is temperature, $z$ is depth into the Earth, and $\alpha$ is the thermal diffusivity. We will model the effects of daily and seasonal variations with a time-dependent boundary condition at $z=0$:

overall, time varying behavior is limited to a certain depth. as you go deeper, temperature fluctuation decreases

$$T(z=0,t) = T_0 + T_1 \sin(\omega_1 t), \tag{2}$$
$$T(z=H,t) = T_0, \tag{3}$$

where we assume that at some depth $z=H$ that the interior temperature is no longer affected by what is happening at the surface, and so the temperature is fixed.

In the limit that $H \to \infty$, this diffusion equation with sinusoidal boundary condition has an exact analytic solution: sin(wt-z/D) addition of phase lag, takes time for heat to diffuse through depth

$$T(z,t) = T_0 + T_1 \sin(\omega_1 t - z/D) \exp(-z/D), \tag{4}$$

exp(-z/D) temperature variation decreases as depth increases

with $D \equiv \sqrt{2\alpha/\omega_1}$. You can verify that this is indeed the solution by substituting into the PDE, and checking that it also satisfies the boundary conditions. The length $D$ is called the "skin depth." Temperature fluctuations propagate as a thermal wave into the Earth, but are damped and only penetrate a few skin depths. The thermal diffusivity for the Earth is approximately $\alpha \approx 10^{-6}$ m$^2$/s. The skin depth is frequency dependent. For daily fluctuations, $D_{daily} \approx 15$ cm, and for yearly fluctuations, $D_{yearly} \approx 3$ m. Thus, short-term variations don't penetrate deeply, while long-term variations do. If you go deep enough into the Earth, the temperature doesn't fluctuate much at all, no matter what is happening at the surface. Note that a similar equation governs how deep fluctuations of a time-varying electric field penetrates into a perfect conductor. modify code to add time varying boundary condition

Your task is to solve this partial differential equation with an *implicit method*, specifically the Crank-Nicolson algorithm. Let's consider seasonal variations, so $\omega_1 = 2\pi$ yr$^{-1}$, $T_0 = 0°$C and $T_1 = 30°$C. Choose $H = 30$ m, which is approximately $10D$. You will need to choose sensible values for $\Delta t$ and $\Delta z$ (Hint: for an implicit method like Crank-Nicolson, a good rule of thumb is that you want $K \equiv \alpha \Delta t/\Delta x^2 \approx 1$). Simulate the temperature for many periods of oscillation. Make a single space-time plot illustrating the evolution of temperature. For example, make a 3D plot with $t$ going into page, $z$ going to the right, and $T$ up and down. Are the amplitudes of fluctuations consistent with depth in terms of skin depths? Are there any phase lags? How deep would you have to go such that the minimum temperature at depth occurs at maximum temperature at the surface, and vice versa? As a bonus, you may want to try to make an animation.

# 2   The Advection Equation

<span style="color:red">allows signals to propagate in one direction
solution is just shifting the wave to the right</span>

The 1D advection equation is:

<span style="color:red">first derivative wrt time —> Crank-Nicolson</span>     <span style="color:red">refer to notes in ilearn</span>

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} \tag{5}$$

where $u$ is some quantity to be advected and $c$ is the advection velocity. For constant $c$, this has an exact solution. Consider the initial condition $u(x, t = 0) = F(x)$. The exact solution for future times is:

$$u(x,t) = F(x - ct), \tag{6}$$

that is, the initial profile is advected to the right with speed $c$. The advection equation is like a "one-way" wave equation, and is a building block to a fully "two-way" wave equation. With constant $c$, the initial profile propagates maintaining its original shape without distortion or dispersion. Your task: Solve with an implicit Crank-Nicolson in time. You should experiment with periodic and transparent boundary conditions. Make a single space-time plot illustrating the propagation of the profile; that is, make a 3D plot with $t$ going into page, $x$ going to the right, and $u$ up and down. As a bonus, you may want to try to make an animation.

# 3   Quantum Particle in a Box: Time-Dependent

The one-dimensional, time-dependent non-relativistic Schrödinger equation for the wave function $\Psi(x,t)$ of a single particle of mass $m$ in a potential $V(x)$ is:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t). \tag{7}$$

Let's use the Hartree atomic units in which $\hbar = m_e = e = 4\pi\varepsilon_0 = 1$. In these units, length is measured in units of the Bohr radius $a_0 = 1$.

(a) Consider an electron in an infinite square well of width $L = 1.0$. The Schrödinger equation is simply:

$$\frac{\partial}{\partial t}\Psi(x,t) = \frac{i}{2}\frac{\partial^2\Psi(x,t)}{\partial x^2}, \tag{8}$$

<span style="color:red">potential goes to infinity at the boundaries, potential =0 inside box. at edge of box, wave function =0</span>

with boundary conditions $\Psi(0,t) = \Psi(L,t) = 0$. This is nearly identical to the thermal diffusion equation, except that it has an imaginary diffusion coefficient (as you will see, that makes all the difference). You will need to modify the arrays and matrices in the thermal diffusion code to be complex valued. For example, let's start off with the wavefunction being a sine function with 3 full periods inside the box:

```
psi = np.zeros([Nx+1,Nt+1]).astype(complex)
psi[:,0] = np.sin(3*2.0*np.pi*x/Lx)
A = np.trapz(psi[:,0]*np.conjugate(psi[:,0]),dx=dx)
psi[:,0] = psi[:,0]/np.sqrt(A)
```

where the last two lines of code normalize the wavefunction so that the total probability is unity (integrating with the trapezoidal rule). Make a graph of the solution at time $t = 0.200$ showing the real part, imaginary part, and square of magnitude of wavefunction. Verify that the square of the magnitude does not change in time (because this wavefunction is an eigenstate). Bonus: make an animation!

(b) Next, consider a wavefunction that is a Gaussian with $\Psi(x,0) = A\exp(-128x^2)$. Make a vertical array of 5 plots showing the wavefunction at times $t = 0.00, 0.04, 0.08, 0.12, 0.16$. Do you notice anything peculiar about the wavefunction at $t = 0.16$? Bonus: make an animation!

(c) Now add an obstacle in the middle of the potential well. (That is, you now have to include $V(x)$.)

# 4   Quantum Particle in a Box: Eigenstates

The one-dimensional, time-independent non-relativistic Schrödinger's equation for the wave function $\psi(x)$ of a single particle of mass $m$ in a potential $V(x)$ is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{9}$$

where $E$ is the total energy. Depending on the shape of the potential, there may be bound states only, scattering states only, or both. In this problem, we will investigate potentials for which there are bound states. When coupled with appropriate boundary conditions, Schrödinger's equation is an eigensystem in which bound states exist only at discrete eigenenergies. Computationally, we will represent the continuous wavefunction as a column vector of values at discrete points: $\psi(x_j) = \psi_j$, for $j = 0, 1, 2, ..., N$. In practice, we specify boundary values for $\psi_0 = \psi_N = 0$, which implies that we are taking the potential at the boundaries to be infinite: $V_0 = V_N \to \infty$. In other words, we are embedding our potential inside an infinite square well. We do not explicitly include equations for the boundaries in our matrix problem. Linear differential operators that operate on the wavefunction become matrices. Using second-order central difference yields a tridiagonal matrix for the second derivative. Scalar multiplication by a known function yields a diagonal matrix with the values of the scalar at the discrete points down the diagonal. Thus:

$$\psi(x) \longrightarrow \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_{N-2} \\ \psi_{N-1} \end{bmatrix}, \quad \frac{d^2}{dx^2} \longrightarrow \frac{1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 \\ 0 & 0 & 0 & \cdots & 1 & -2 \end{bmatrix}, \quad V(x) \longrightarrow \begin{bmatrix} V_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & V_2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & V_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & V_{N-2} & 0 \\ 0 & 0 & 0 & \cdots & 0 & V_{N-1} \end{bmatrix} \tag{10}$$

The Schrödinger's equation can then be written in matrix form:

$$\mathbf{H}\,|\psi\rangle = \lambda\,|\psi\rangle. \tag{11}$$

Let's use the Hartree atomic units in which $\hbar = m_e = e = 4\pi\varepsilon_0 = 1$. In these units, length is measured in units of the Bohr radius $a_0 = 1$, and energy is measured in units of "hartrees": $1\ E_h \equiv \hbar^2/(m_e a_0^2)$. You have been given Python code to find the eigenenergies and eigenfunctions for an electron in an infinite square well of width $L = \pi$. The eigenenergies with then be $E_n = n^2/2$. Play around with this code to make sure you understand how to find eigenvalues and eigenvectors.

(a) Let's perturb the square well with a Gaussian perturbation: $V(x) = 100\exp(-64x^2)$. Compute the energy shifts for the first 6 modes and graph their eigenfunctions. Do you notice a difference between even and odd modes? Be sure to discuss in your caption.

(b) Consider the case of the quantum harmonic oscillator: $V(x) = m\omega_0^2 x^2/2$. In computational units, let's choose $\omega_0 = 2.0$. There are more clever ways of handling the boundary conditions, but for simplicity, we will embed our QHO in an infinite square well. Let's choose $L = 10.0$. This will distort the eigenmodes that have turning points near the boundaries of the well. For the matrix sizes, let's choose $N = 1001$ (999 without boundaries). Compute the first 6 eigenvalues and eigenvectors. Then find the largest eigenvalue for which the result is still correct within 10%.

(c) Now create your own potential and compute some eigenvalues and eigenvectors!