PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF Olin 103

Notes on Lecture 35: Chap. 11 in F&W

Heat conduction

1. Basic equations
2. Boundary value problems

In today's lecture we will take a quick look at heat transfer following Chapter 11 of your textbook.

33	Fri, 11/12/2021	Chap. 10	Surface waves in fluids
34	Mon, 11/15/2021	Chap. 10	Surface waves in fluids; soliton solutions
35	Wed, 11/17/2021	Chap. 11	Heat conduction
36	Fri, 11/19/2021	Chap. 12	Viscous effects on hydrodynamics
	Mon, 11/22/2021		Presentations
	Wed, 11/24/2021		Thanksgiving
	Fri, 11/26/2021		Thanksgiving
37	Mon, 11/29/2021	Chap. 13	Elasticity
38	Wed, 12/01/2021	Chap. 1-13	Review
39	Fri, 12/03/2021	Chap. 1-13	Review

Schedule.

Schedule for Monday, November 22, 2021

Time	Name	Topic
10:00-10:20	Owen	
10:20-10:40	Manikata	
10:40-11:00	Wells	
11:00-11:20	Can	
11:20-11:40	Ramesh	

Fill in topic!

PHYSICS COLLOQUIUM

4 PM Olin 101 & zoom

THURSDAY

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NOVEMBER 18, 2021

"Breaking Ultrathin Ionic Wires in LNNano"

This talk is divided into two parts.

In the first part, I´ll briefly describe the Brazilian Nanotechnology National Laboratory (LNNano), an open facility for research and innovation in the field of nanoscience and nanotechnology located in Campinas, Brazil, in the same campus as 3 other National Laboratories which include Sirius, a 4th generation synchrotron facility.

In the second part, I´ll discuss our recent joint theory/experiment work on the formation and rupture of monatomic ZrO2 wires.

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Federal University of Rio de Janeiro
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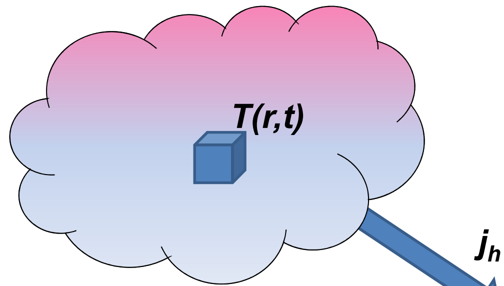
Conduction of heat



Enthalpy of a system at constant pressure p

non uniform temperature $T(\mathbf{r},t)$

mass density ρ and heat capacity c_p

$$H = \int_V \rho c_p \left(T(\mathbf{r},t) - T_0\right) d^3r + H_0\left(T_0, p\right)$$

Enthalpy as a measure of heat of a system at constant pressure in terms of the heat capacity of the material.

Note that in this treatment we are considering a system at constant pressure p

Notation: Heat added to system -- $dQ = TdS$

External work done on system -- $dW = -pdV$

Internal energy -- $dE = dQ + dW = TdS - pdV$

Entropy -- dS

Enthalpy -- $dH = d(E + pV) = TdS + Vdp$

Heat capacity at constant pressure:

$$C_p \equiv \left(\frac{dQ}{dT}\right)_p = \left(\frac{\partial H}{\partial T}\right)_p = T\left(\frac{\partial S}{\partial T}\right)_p$$

$$C_p = \int \rho c_p d^3r$$

More generally, note that c_p can depend on T; we are assuming that dependence to be trivial.

Some notations and concepts from thermodynamics.

Conduction of heat -- continued

$$H = \int_V \rho c_p \left(T(\mathbf{r},t) - T_0\right) d^3r + H_0(T_0, p)$$

Time rate of change of enthapy:

$$\frac{dH}{dt} = \int_V \rho c_p \frac{\partial T(\mathbf{r},t)}{\partial t} d^3r = -\int_A \mathbf{j}_h \cdot d\mathbf{A} + \int_V \rho \dot{q} d^3r$$

heat flux

heat source

$$\rho c_p \frac{\partial T(\mathbf{r},t)}{\partial t} = -\nabla \cdot \mathbf{j}_h + \rho \dot{q}$$

Now consider how the enthalpy of a system may change in time. The temperature may change, there may be heat flux, and there may be a source or sink for heat flow.

Conduction of heat -- continued

$$\rho c_p \frac{\partial T(\mathbf{r},t)}{\partial t} = -\nabla \cdot \mathbf{j}_h + \rho \dot{q}$$

$$\text{Empirically:} \quad \mathbf{j}_h = -k_{th} \nabla T(\mathbf{r},t)$$

$$\Rightarrow \frac{\partial T(\mathbf{r},t)}{\partial t} = \kappa \nabla^2 T(\mathbf{r},t) + \frac{\dot{q}}{c_p}$$

$$\kappa \equiv \frac{k_{th}}{\rho c_p}$$ thermal diffusivity

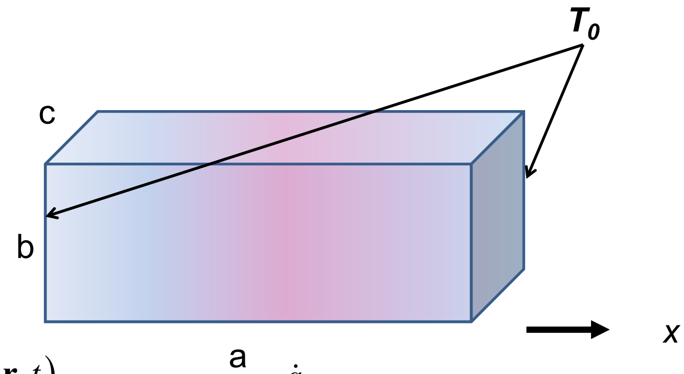
https://www.engineersedge.com/heat_transfer/thermal_diffusivity_table_13953.htm

Typical values (m^2/s)

Air	$2x10^{-5}$
Water	$1x10^{-7}$
Copper	$1x10^{-4}$

In order to relate these quantities, we need to know how enthalpy is related to temperature and we will use the empirical relations based on observation that heat flux is proportional to the gradient of temperature. The Thermal diffusivity coefficient is highly dependent on the material as seen in this short list taken from the internet.

Boundary value problems for heat conduction



$$\frac{\partial T(\mathbf{r},t)}{\partial t} - \kappa\nabla^2 T(\mathbf{r},t) = \frac{\dot{q}}{c_p}$$

Without source term: $\frac{\partial T(\mathbf{r},t)}{\partial t} - \kappa\nabla^2 T(\mathbf{r},t) = 0$

Example with boundary values: $T(0,y,z,t) = T(a,y,z,t) = T_0$

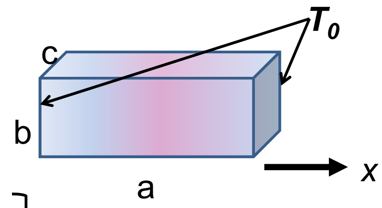
Example boundary value problem which we will solve in the case that the source term is zero.

Have you ever encountered the following equation in other contexts and if so where?

$$\frac{\partial T(\mathbf{r},t)}{\partial t} - \kappa\nabla^2 T(\mathbf{r},t) = 0$$

Boundary value problems for heat conduction

$$\frac{\partial T(\mathbf{r},t)}{\partial t} - \kappa\nabla^2 T(\mathbf{r},t) = 0$$



$$T(0,y,z,t) = T(a,y,z,t) = T_0$$

$$\frac{\partial T(x,0,z,t)}{\partial y} = \frac{\partial T(x,b,z,t)}{\partial y} = 0$$

$$\frac{\partial T(x,y,0,t)}{\partial z} = \frac{\partial T(x,y,c,t)}{\partial z} = 0$$

Assuming thermally insulated boundaries

Separation of varables : $T(x,y,z,t) = T_0 + X(x)Y(y)Z(z)e^{-\lambda t}$

Let $\frac{d^2X}{dx^2} = -\alpha^2 X \quad \frac{d^2Y}{dy^2} = -\beta^2 Y \quad \frac{d^2Z}{dz^2} = -\gamma^2 Z$

$$\Rightarrow -\lambda + \kappa\left(\alpha^2 + \beta^2 + \gamma^2\right) = 0$$

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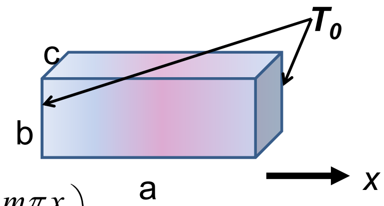
Using separation of variables to solve the problem.

Boundary value problems for heat conduction



$$T(x,y,z,t) = T_0 + X(x)Y(y)Z(z)e^{-\lambda t}$$

$$X(0) = X(a) = 0 \qquad \Rightarrow X(x) = \sin\left(\frac{m\pi x}{a}\right)$$

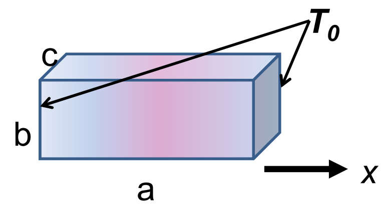
$$\frac{dY(0)}{dy} = \frac{dY(b)}{dy} = 0 \qquad \Rightarrow Y(y) = \cos\left(\frac{n\pi y}{b}\right)$$

$$\frac{dZ(0)}{dz} = \frac{dZ(c)}{dz} = 0 \qquad \Rightarrow Z(z) = \cos\left(\frac{p\pi z}{c}\right)$$

$$-\lambda_{nmp} + \kappa\left(\left(\frac{n\pi}{a}\right)^2 + \left(\frac{m\pi}{b}\right)^2 + \left(\frac{p\pi}{c}\right)^2\right) = 0$$

Some details for this case.

Boundary value problems for heat conduction



Full solution:

$$T\left(x,y,z,t\right)=T_0+\sum_{nmp} C_{nmp}\sin\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right)\cos\left(\frac{p\pi z}{c}\right)e^{-\lambda_{mnp}t}$$

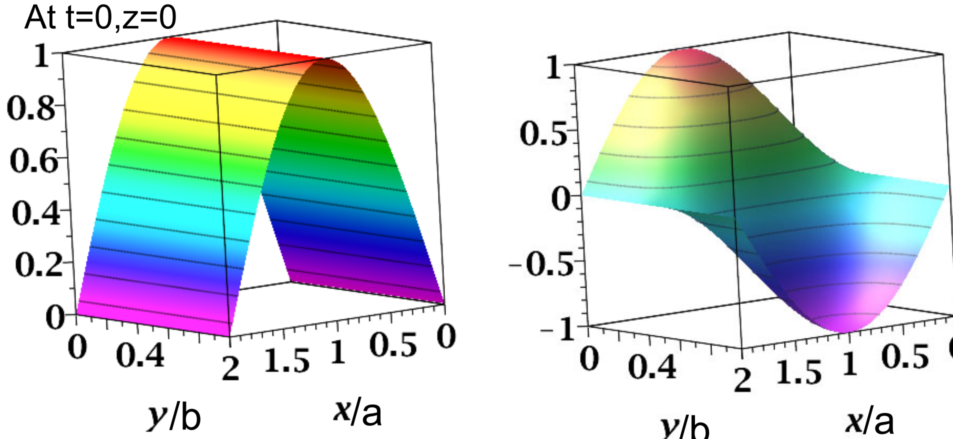
$$\lambda_{nmp}=\kappa\left(\left(\frac{n\pi}{a}\right)^2+\left(\frac{m\pi}{b}\right)^2+\left(\frac{p\pi}{c}\right)^2\right)$$

More details.

Full solution:

$$T(x,y,z,t) = T_0 + \sum_{nmp} C_{nmp} \sin\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right)\cos\left(\frac{p\pi z}{c}\right)e^{-\lambda_{mnp}t}$$

At t=0,z=0

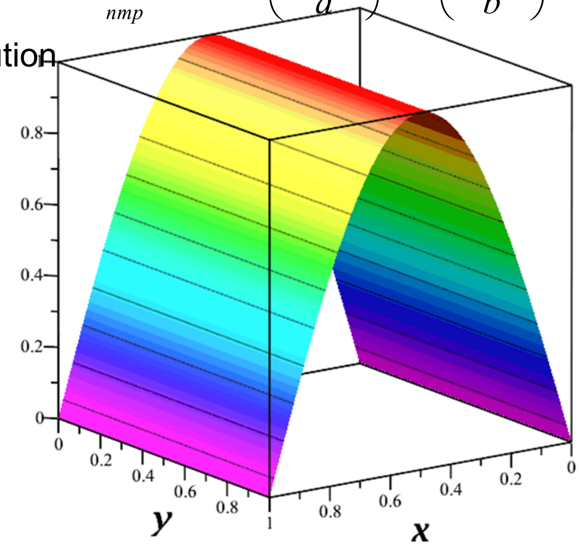


$m=1, n=0, p=0$ $\qquad$ $m=1, n=1, p=0$

Full solution:

$$T\left(x,y,z,t\right)=T_0+\sum_{nmp}C_{nmp}\sin\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right)\cos\left(\frac{p\pi z}{c}\right)e^{-\lambda_{mnp}t}$$

Time evolution
nmp=100
at *z=0*



Visualization of the time evolution.

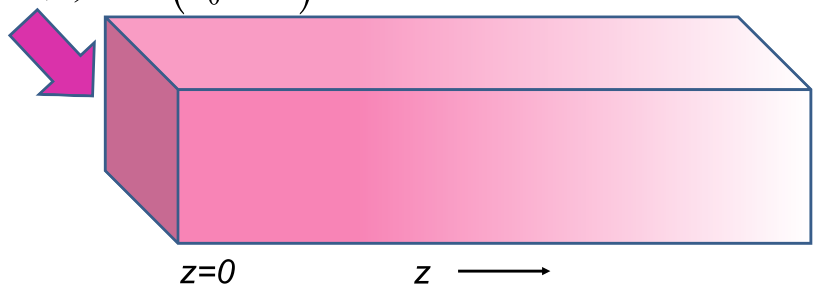
What real system could have such a temperature distribution?

Comment – While one can imagine that the boundary conditions can be readily realized, the single normal mode patterns are much harder. On the other hand, we see that the lowest values of lambda have the longest time constants.

Oscillatory thermal behavior

Here we assume that the spatial variation is along z

$$T(z=0,t) = \Re\left(T_0 e^{-i\omega t}\right)$$



$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial z^2}$$

Assume: $T(z,t) = \Re\left(f(z) e^{-i\omega t}\right)$

$$(-i\omega) f = \kappa \frac{d^2 f}{dz^2}$$

Let $f(z) = Ae^{\alpha z}$

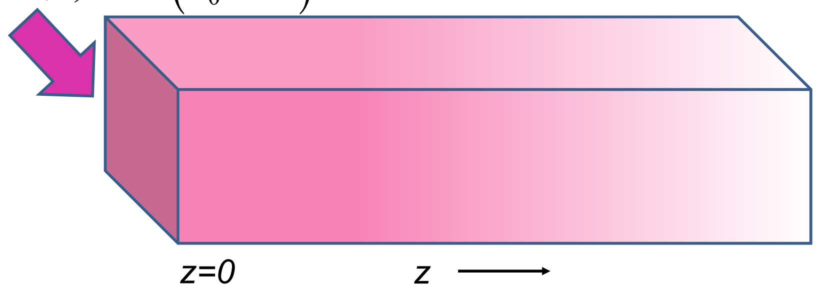
$$\alpha^2 = -\frac{i\omega}{\kappa} = e^{3i\pi/2} \frac{\omega}{\kappa}$$

$$\alpha = \pm(1-i)\sqrt{\frac{\omega}{2\kappa}}$$

Now consider an oscillatory solutions.

Oscillatory thermal behavior -- continued

$$T(z=0,t)=\Re\left(T_0 e^{-i\omega t}\right)$$



$$T(z,t)=\Re\left(A e^{\pm(1-i)z/\delta} e^{-i\omega t}\right)$$

where $\delta \equiv \sqrt{\dfrac{2\kappa}{\omega}}$

Physical solution: $T(z,t)=T_0 e^{-z/\delta}\cos\left(\dfrac{z}{\delta}-\omega t\right)$

Analysis of solution.

$$T(z,t) = T_0 e^{-z/\delta} \cos\left(\frac{z}{\delta} - \omega t\right)$$

$t = 0.$

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Animation of solution.

Does this expression say the temperature transmits along the z axis?

Comment – In this case, our setup approximates trivial variation in the x-y plane so that all variation is along z. The spatial form along z with oscillating boundary condition at z=0 is a result of the form of the heat equation.

Initial value problem in an infinite domain; Fourier transform

$$\frac{\partial T(\mathbf{r},t)}{\partial t} - \kappa \nabla^2 T(\mathbf{r},t) = 0$$

$$T(\mathbf{r},0) = f(\mathbf{r})$$

$$\text{Let}: \quad \tilde{T}(\mathbf{q},t) = \int d^3 r e^{-i\mathbf{q}\cdot\mathbf{r}} T(\mathbf{r},t)$$

$$\tilde{f}(\mathbf{q}) = \int d^3 r e^{-i\mathbf{q}\cdot\mathbf{r}} f(\mathbf{r})$$

$$\Rightarrow \tilde{T}(\mathbf{q},0) = \tilde{f}(\mathbf{q})$$

$$\Rightarrow \frac{\partial \tilde{T}(\mathbf{q},t)}{\partial t} = -\kappa q^2 \tilde{T}(\mathbf{q},t)$$

$$\tilde{T}(\mathbf{q},t) = \tilde{T}(\mathbf{q},0) e^{-\kappa q^2 t}$$

Now consider an initial value problem.

Initial value problem in an infinite domain; Fourier transform

$$\widetilde{T}(\mathbf{q},t) = \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} T(\mathbf{r},t) \qquad \Rightarrow T(\mathbf{r},t) = \frac{1}{(2\pi)^3}\int d^3q e^{i\mathbf{q}\cdot\mathbf{r}} \widetilde{T}(\mathbf{q},t)$$

$$\widetilde{T}(\mathbf{q},t) = \widetilde{T}(\mathbf{q},0) e^{-\kappa q^2 t}$$

$$T(\mathbf{r},t) = \frac{1}{(2\pi)^3}\int d^3q e^{i\mathbf{q}\cdot\mathbf{r}} \widetilde{T}(\mathbf{q},0) e^{-\kappa q^2 t}$$

$$\widetilde{T}(\mathbf{q},0) = \widetilde{f}(\mathbf{q}) = \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} f(\mathbf{r})$$

$$T(\mathbf{r},t) = \int d^3r' G(\mathbf{r}-\mathbf{r}',t) T(\mathbf{r}',0)$$

$$\text{with } \; G(\mathbf{r}-\mathbf{r}',t) \equiv \frac{1}{(2\pi)^3}\int d^3q e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} e^{-\kappa q^2 t}$$

Using Green's functions to analyze the results.

Initial value problem in an infinite domain; Fourier transform

$$T(\mathbf{r},t) = \int d^3r' \, G(\mathbf{r}-\mathbf{r}',t) T(\mathbf{r}',0)$$

$$\text{with} \quad G(\mathbf{r}-\mathbf{r}',t) \equiv \frac{1}{(2\pi)^3} \int d^3q \, e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} e^{-\kappa q^2 t}$$

$$G(\mathbf{r}-\mathbf{r}',t) = \frac{1}{(4\pi\kappa t)^{3/2}} e^{-|\mathbf{r}-\mathbf{r}'|^2/(4\kappa t)}$$

Some details.

Heat equation in half-space

$$\frac{\partial T(\mathbf{r},t)}{\partial t} - \kappa\nabla^2 T(\mathbf{r},t) = 0$$

$T(\mathbf{r},t) \Rightarrow T(z,t)$ with initial and boundary values:

$$T(z,t) \equiv 0 \quad \text{for } z < 0$$

$$T(z,0) = 0 \quad \text{for } z > 0$$

$$T(0,t) = T_0 \quad \text{for } t \geq 0$$

$$\text{Solution}: \quad T = T_0 \,\text{erfc}\left(\frac{z}{2\sqrt{\kappa t}}\right)$$

$$\text{where } \text{erfc}(x) \equiv \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du$$

For half space boundary.

Your question -- Can you explain the erf function. I've never really understood it. I'm not sure I've actually ever had someone explain it. I've just seen it appear in places before. https://dlmf.nist.gov/7

§7.2(i) Error Functions

7.2.1 $$\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2}\, dt,$$

7.2.2 $$\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2}\, dt = 1 - \operatorname{erf} z,$$

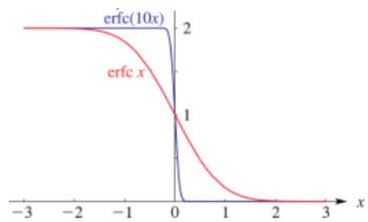


Figure 7.3.1: Complementary error functions $\operatorname{erfc} x$ and $\operatorname{erfc}(10x)$, $-3 \le x \le 3$.

Heat equation in half-space -- continued

$$\frac{\partial T(z,t)}{\partial t} - \kappa \frac{\partial^2 T(z,t)}{\partial z^2} = 0$$

Solution : $T = T_0 \operatorname{erfc}\left(\frac{z}{2\sqrt{\kappa t}}\right)$

where $\operatorname{erfc}(x) \equiv \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du$

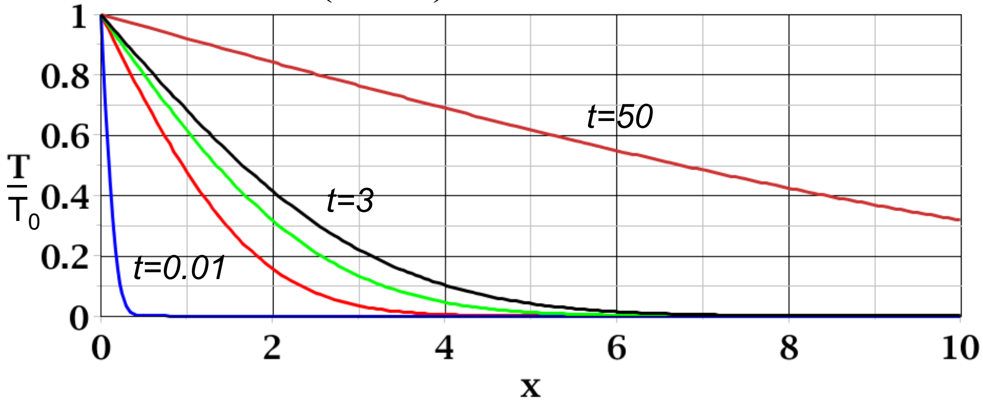
Note that $\frac{d \operatorname{erfc}(x)}{dx} = \frac{d}{dx} \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du = -\frac{2}{\sqrt{\pi}} e^{-x^2}$

$$\frac{\partial}{\partial t} \operatorname{erfc}\left(\frac{z}{2\sqrt{\kappa t}}\right) = \frac{2}{\sqrt{\pi}} e^{-\left(z^2/(4\kappa t)\right)} \left(\frac{z}{4\sqrt{\kappa t^3}}\right)$$

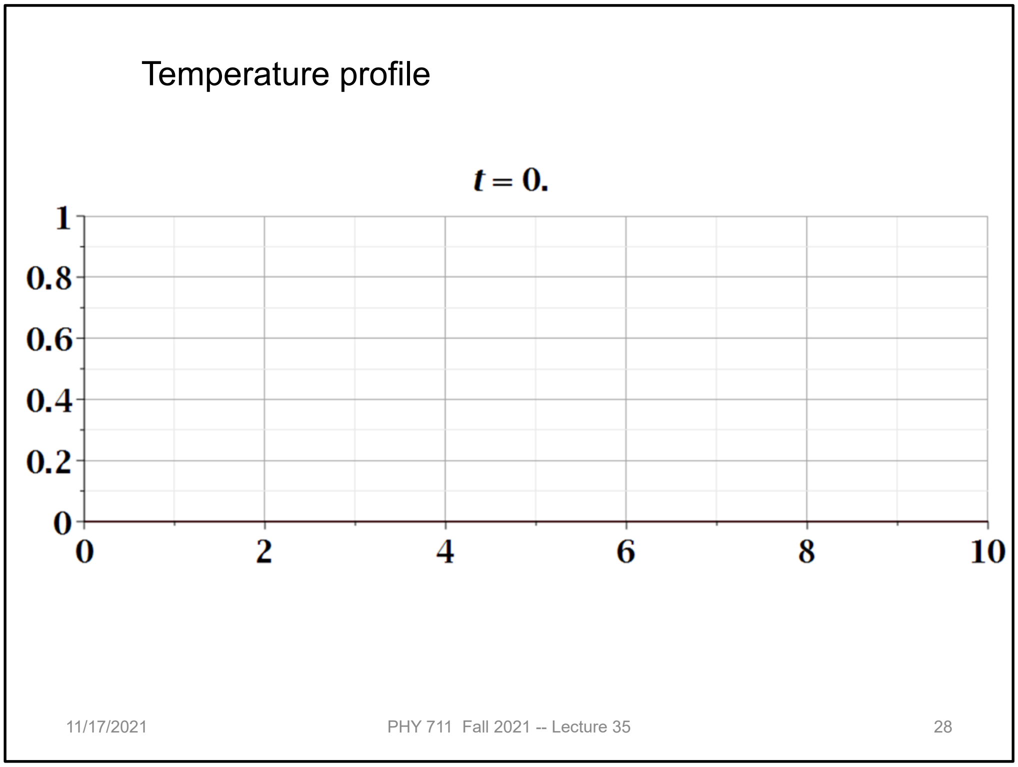
$$\frac{\partial^2}{\partial z^2} \operatorname{erfc}\left(\frac{z}{2\sqrt{\kappa t}}\right) = \frac{2}{\sqrt{\pi}} e^{-\left(z^2/(4\kappa t)\right)} \left(\frac{z}{4\kappa\sqrt{\kappa t^3}}\right)$$

Some details.

$$T = T_0 \ \mathrm{erfc}\left(\frac{z}{2\sqrt{\kappa t}}\right)$$



Plots of solution at various times.


Temperature profile
t = 0.
1
0.8
0.6
0.4
0.2
0
0
2
4
6
8
10
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Animation.