

Phys 366

Lecture 22-23a

Partial differential equations. I

Where do the big-time PDEs come from?

Laplacian $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ 1d
2d
3d

① Electrostatics: $\nabla \cdot \vec{E} = 4\pi \rho$ $\Rightarrow \nabla^2 \Phi = -4\pi \rho$
charge density Poisson equation
 $\nabla \times \vec{E} = 0 \Rightarrow \vec{E} = -\nabla \Phi$ $\rho=0$: Laplacian
electric field electrostatic potential

Poisson solution: $\Phi(\vec{r}) = \int d^3r' \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|}$

$\nabla^2 \left(\frac{1}{|\vec{r} - \vec{r}'|} \right) = -4\pi \delta(\vec{r} - \vec{r}')$

Theme: Green function. Works for linear equations (superposition)

② Conservation laws

② $\frac{d}{dt} \int_V d\tau n = - \oint_S \vec{F} \cdot d\vec{a} + \int_V d\tau S$ $[F] = \frac{[n]L}{T}$
number density or concentration of something number current density of the something
Source or sink rate per unit volume of the something

Differential form: $\frac{\partial n}{\partial t} = -\nabla \cdot \vec{F} + S$

Phenomenology: $\vec{F} = -\mathcal{K} \nabla n$ $[\mathcal{K}] = \frac{[F]L}{[n]} = \frac{L^2}{T}$
transport coefficient

$\frac{\partial n}{\partial t} = \mathcal{K} \nabla^2 n + S$

③ What if n is the internal energy density u ? $u = c_V T$, $\vec{F} = -\mathcal{K} \nabla T$ thermal conductivity
specific heat
 $c_V \frac{\partial T}{\partial t} = \mathcal{K} \nabla^2 T + S$ $[c_V] = \frac{E}{L^3 K}$ $[\mathcal{K}] = \frac{F}{LTK}$

Diffusion equation (with source)

$[\mathcal{K}/c_V] = \frac{L^2}{T}$

$\nabla^2 f - \frac{1}{\mathcal{K}} \frac{\partial f}{\partial t} = -\frac{S}{\mathcal{K}} = -S$
material property

Diffusion equations arise whenever a conserved quantity flows in response to a gradient in the quantity.

Wave equation: $\nabla^2 f - \frac{1}{v^2} \frac{\partial^2 f}{\partial t^2} = s$ ← source

① String under tension: $\lambda \frac{\partial^2 f}{\partial z^2} = T \frac{\partial^2 f}{\partial x^2} + f$

$$\frac{\partial^2 f}{\partial x^2} - \frac{1}{v^2} \frac{\partial^2 f}{\partial t^2} = \frac{f}{T} = s$$

↑ external force per length

$$v^2 = T/\lambda$$

② Pressure sound waves

$$\rho_0 \frac{\partial^2 \vec{\xi}}{\partial t^2} = -\nabla p = \gamma p_0 \nabla (\nabla \cdot \vec{\xi})$$

$$\nabla (\nabla \cdot \vec{\xi}) - \frac{1}{v^2} \frac{\partial^2 \vec{\xi}}{\partial t^2} = 0,$$

$$v^2 = \gamma p_0 / \rho_0$$

Taking the curl of this equation implies

$$\frac{\partial^2 (\nabla \times \vec{\xi})}{\partial t^2} = 0$$

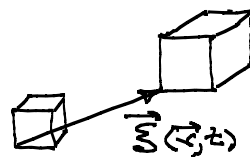
So $\nabla \times \vec{\xi}$ doesn't participate in the wave action and can be set to zero. $\nabla \times \vec{\xi} = 0$ defines a longitudinal wave, i.e., one where $\vec{\xi}$ is along the direction of propagation. Taking the divergence gives

$$\nabla^2 (\nabla \cdot \vec{\xi}) - \frac{1}{v^2} \frac{\partial^2 (\nabla \cdot \vec{\xi})}{\partial t^2} = 0 \quad \text{wave equation for } \nabla \cdot \vec{\xi}$$

OR use $\nabla^2 \vec{A} = \nabla (\nabla \cdot \vec{A}) - \nabla \times (\nabla \times \vec{A})$ to write

$$\nabla^2 \vec{\xi} - \frac{1}{v^2} \frac{\partial^2 \vec{\xi}}{\partial t^2} = 0, \quad \nabla \times \vec{\xi} = 0$$

③ Maxwell equations give wave equations with sources for the scalar and vector potentials.



$$pV^\gamma = \text{constant} \quad \gamma = \frac{c_p}{c_v}$$

$$\Delta p V_0^\gamma + \gamma p_0 V_0^{\gamma-1} \Delta V = 0$$

$$\Delta p = -\gamma p_0 \frac{\Delta V}{V} = -\gamma p_0 \nabla \cdot \vec{\xi}$$

$$\Rightarrow p = p_0 - \underbrace{\gamma p_0 \nabla \cdot \vec{\xi}}_{\text{changes in pressure due to compression and expansion in the gas}}$$

equilibrium pressure

(3)

④ Helmholtz equation: FT of wave equation with respect to time.

$$\nabla^2 f - \frac{1}{v^2} \frac{\partial^2 f}{\partial t^2} = 0$$

$$f(\vec{r}, t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{f}(\vec{r}, \omega) e^{-i\omega t}$$

$$0 = \nabla^2 f - \frac{1}{v^2} \frac{\partial^2 f}{\partial t^2} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left(\nabla^2 \tilde{f} + \frac{\omega^2}{v^2} \tilde{f} \right)$$

$$\nabla^2 \tilde{f} + k^2 \tilde{f} = 0, \quad k = \omega/v$$

⑤ Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) \psi = i\hbar \frac{\partial \psi}{\partial t}$$

Where does this come from? De Broglie waves: $E = \hbar\omega$, $\vec{p} = \hbar\vec{k}$

$$\text{FT: } E = \hbar\omega \longrightarrow E = i\hbar \frac{\partial}{\partial t}$$

$$\vec{p} = \hbar\vec{k} \longrightarrow \vec{p} = \frac{\hbar}{i} \nabla$$

$$\underbrace{\left(\frac{\vec{p} \cdot \vec{p}}{2m} + V(\vec{r}) \right)}_{\text{Hamiltonian } H} \psi = E \psi \iff \left(-\frac{\hbar^2}{2m} \nabla \cdot \nabla + V(\vec{r}) \right) \psi = i\hbar \frac{\partial \psi}{\partial t}$$

Hamiltonian H

$H = -\frac{\hbar^2}{2m} \nabla^2 + V$ is a Hermitian operator. What the heck could that mean? We have discussed the inner product on the space of square-integrable functions,

$$\int d^3r \phi^*(\vec{r}) \psi(\vec{r}) = (\phi, \psi) = \langle \phi | \psi \rangle.$$

So Hermiticity means

$$\langle \phi | H | \psi \rangle = \langle \psi | H | \phi \rangle^* \text{ or } (\phi, H\psi) = (H\phi, \psi) \text{ or}$$

$$\int d^3r \phi^*(\vec{r}) H\psi(\vec{r}) = \int d^3r (H\phi)^*(\vec{r}) \psi(\vec{r})$$

Does it work? It's obvious it works for $\nabla(\vec{r})$, so we only need to show it for ∇^2 . ④

$$\begin{aligned}\int d^3r \phi^* \nabla \cdot \nabla \psi &= \int d^3r \nabla \cdot (\phi^* \nabla \psi) - \int d^3r \nabla \phi^* \cdot \nabla \psi \\ &= - \int d^3r \nabla \phi^* \cdot \nabla \psi + \oint_S \phi^* \nabla \psi \cdot \vec{da}\end{aligned}$$

$$\begin{aligned}\int d^3r (\nabla \cdot \nabla \phi)^* \psi &= \int d^3r \nabla \cdot (\psi \nabla \phi^*) - \int d^3r \nabla \phi^* \cdot \nabla \psi \\ &= - \int d^3r \nabla \phi^* \cdot \nabla \psi + \oint_S \psi \nabla \phi^* \cdot \vec{da}\end{aligned}$$

$$\text{So } \int d^3r \phi^* \nabla^2 \psi - \int d^3r (\nabla^2 \phi)^* \psi = \underbrace{\oint_S (\phi^* \nabla \psi - \psi \nabla \phi^*) \cdot \vec{da}} = 0$$

The physics of the problem imposes appropriate boundary conditions to make this vanish, either ψ or $\nabla \psi \cdot \hat{n}$ vanishes on S or some combination of these.

Theme: Hermitian operators and complete sets of their eigenfunctions.
Eigenvalue problems.

This allows us to treat the Schrödinger equation as an operator equation,

$$H|\psi\rangle = i\hbar \frac{d|\psi\rangle}{dt} \longleftrightarrow \left(-\frac{\hbar^2}{2m} \nabla^2 + V\right)\psi = i\hbar \frac{\partial \psi}{\partial t}$$

position representation

$|\vec{r}\rangle$ is the position eigenstate

to solve it formally as

$$|\psi(t)\rangle = \underbrace{e^{-iHt/\hbar}}_{U(t) \leftarrow \text{unitary evolution operator}} |\psi(0)\rangle \rightarrow \psi(\vec{r}, t) = \int d^3r' \underbrace{\langle \vec{r} | U(t) | \vec{r}' \rangle}_{\text{propagator } G(\vec{r}, t; \vec{r}')} \psi(\vec{r}', 0)$$

This is a temporal Green function

and to solve it in principle in terms of the energy eigenstates,

$$\begin{array}{ccc} H|E_n\rangle = E_n|E_n\rangle & \longrightarrow & \left(-\frac{\hbar^2}{2m} \nabla^2 + V\right)\psi_n(\vec{r}) = E_n\psi_n(\vec{r}) \\ \uparrow & & \uparrow \\ \text{energy (stationary) state} & & \text{energy eigenfunction} \end{array}$$

The energy eigenstates are a complete, orthonormal set:

Orthonormality: $\langle E_n | E_m \rangle = \int d^3r \psi_n^*(\vec{r}) \psi_m(\vec{r}) = \delta_{nm}$

Completeness: $\sum_n |E_n\rangle \langle E_n| = I \leftrightarrow \sum_n \psi_n(\vec{r}) \psi_n^*(\vec{r}') = \delta^3(\vec{r} - \vec{r}')$

Energy-eigenstate solution of the dynamics:

$$U(t) = \sum_n e^{-iE_n t/\hbar} |E_n\rangle \langle E_n|$$

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle = \sum_n e^{-iE_n t/\hbar} |E_n\rangle \langle E_n| \psi(0)\rangle$$

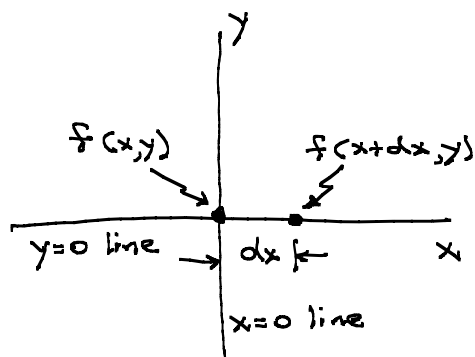
Propagator: $\langle \vec{r} | U(t) | \vec{r}' \rangle = \sum_n e^{-iE_n t/\hbar} \psi_n(\vec{r}) \psi_n^*(\vec{r}')$

$$\psi(\vec{r}, t) = \sum_n e^{-iE_n t/\hbar} \psi_n(\vec{r}) \underbrace{\int d^3r' \psi_n^*(\vec{r}') \psi(\vec{r}', 0)}_{c_n = \langle E_n | \psi(0) \rangle}$$

Partial derivatives:

Function $f(x, y, z)$

$$\frac{\partial f}{\partial x} = \frac{f(x+dx, y, z) - f(x, y, z)}{dx} = \left(\frac{\partial f}{\partial x} \right)_{y, z}$$



Taking a partial derivative with respect to a variable requires knowing which other variables are held fixed. Sometimes we denote this, but usually it is left to context, and this can cause confusion.

① Change of variables: $x_1, \dots, x_N$
 $y_1, \dots, y_N$

$$\frac{\partial f}{\partial y_j} = \sum_{k=1}^N \frac{\partial f}{\partial x_k} \frac{\partial x_k}{\partial y_j}$$

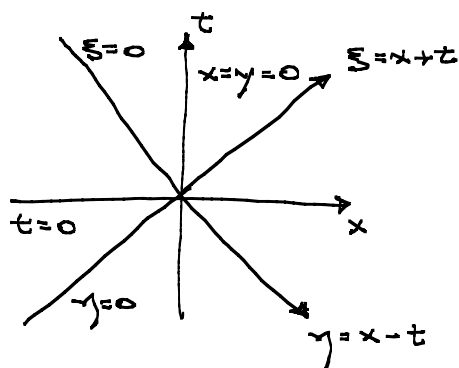
Single variable

$$\frac{df}{dy} = \frac{df}{dx} \frac{dx}{dy}$$

Jacobian matrix
 M_{kj}

The Jacobian matrix describes a linear transformation of the partial derivatives. If the transformation of the variables is itself linear, e.g., an orthogonal transformation, then the Jacobian is a constant, independent of position. Otherwise, the Jacobian is still a linear transformation of partial derivatives, but it changes from place to place.

Example:



$$\xi = x + z \quad x = \frac{1}{2}(\xi + \eta)$$

$$\eta = x - z \quad z = \frac{1}{2}(\xi - \eta)$$

$$\frac{\partial f}{\partial \xi} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial \xi} = \frac{1}{2} \left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial z} \right)$$

$$\frac{\partial f}{\partial \eta} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial \eta} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial \eta} = \frac{1}{2} \left(\frac{\partial f}{\partial x} - \frac{\partial f}{\partial z} \right)$$

But, what if we change to variables $y = x$ $x = y$
 $\xi = x + z$ $z = \xi - y$

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial y} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial y} = \frac{1}{2} \left(\frac{\partial f}{\partial x} - \frac{\partial f}{\partial z} \right)$$

$$\frac{\partial f}{\partial \xi} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial \xi} = \frac{\partial f}{\partial z}$$

$\frac{\partial f}{\partial y} \neq \frac{\partial f}{\partial x}$ even though $x=y$;
 that's because $z \neq \xi$.

② Extrema

Function $f(x)$ of one variable: $f'(x_0) = 0$ $\begin{cases} f''(x_0) > 0 & \text{maximum} \\ f''(x_0) = 0 & \text{depends on} \\ f''(x_0) < 0 & \text{minimum} \end{cases}$
 extremum

Function $f(x, y)$ of two variables:

$$0 = \frac{\partial f}{\partial x} \Big|_{(x_0, y_0)} = \frac{\partial f}{\partial y} \Big|_{(x_0, y_0)} \leftarrow \text{extremum}$$

There are more possibilities here. Suppose $x_0 = y_0 = 0$. Near $x_0 = y_0 = 0$, f looks like

$$f(x, y) = f_0 + \frac{1}{2} \left(\underbrace{\frac{\partial^2 f}{\partial x^2}}_a x^2 + \underbrace{\frac{\partial^2 f}{\partial y^2}}_b y^2 + 2 \underbrace{\frac{\partial^2 f}{\partial x \partial y}}_c xy \right)$$

evaluated at $x=y=0$

$$= f_0 + \frac{1}{2} \underbrace{\begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} a & c \\ c & b \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}}_{\text{quadratic form}}$$

Suppose $c = 0$:

① $a, b > 0$: Minimum

② $a, b < 0$: Maximum

③ $a > 0, b < 0$ or $a < 0, b > 0$: Saddle point

$a = 0$ or $b = 0$: depends on higher derivatives

Suppose $a = -b$; let $\xi = x + y, \eta = x - y$

$$f = f_0 + \frac{1}{2} a \underbrace{(x^2 - y^2)}_{(x+y)(x-y)} = f_0 + \frac{1}{2} a \xi \eta = f_0 + \frac{1}{4} a (\xi \eta) \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}$$

It is not the diagonal elements that count; it's eigenvalues of the quadratic form.

Generally, if $\left. \frac{\partial f}{\partial x_j} \right|_0 = 0$ for all j ,

$$f = f_0 + \underbrace{\frac{1}{2} \sum_{j,k} (x_j - x_{j0}) \underbrace{\frac{\partial^2 f}{\partial x_j \partial x_k} \bigg|_0}_{M_{jk}} (x_k - x_{k0})}_{\text{quadratic form}}$$

① All eigenvalues of $M > 0$: minimum

M is a positive-definite matrix

② All eigenvalues of $M < 0$: maximum

M is a negative-definite matrix

③ Some eigenvalues of $M > 0$, others < 0 : saddle point

If any eigenvalues are 0, you need to look at higher derivatives.