Tutorial 0:Prerequisite

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1. Integrals of Derivatives.

For one variable, we have fundamental theorem of calculs. Then if f is differential in $[a, b]$, we have

$$f(b) - f(a) = \int_a^b f'(x)dx$$

For two variables, we introduce the Green's Formla. For high variables, Gauss Formula or Divergence Theorem.

Green's Fromula.

Let D be a bounded plane domain with a piecewise C^1 boundary curve $C = bdyD$. Consider C to be parametrized so that it is traversed once with D on the left. Let $p(x, y)$ and $q(x, y)$ be any C^1 functions defined on $\overline{D} = D \cup C$. Then

$$\iint_D (q_x - p_y)dxdy = \int_C pdx + qdy.$$

Divergence Theorem:

Let D be a bounded spatial domian with a piecewise C^1 boundary surface S. Let $\vec{n}$ be the unit outward normal vector on S. Let $f(x)$ be any C^1 vector field on $\overline{D} = D \cup S$. Then

$$\iiint_D \nabla \cdot f dx = \iint_S f \cdot \vec{n}.$$

2.Derivatives of integrals.

Thm 1 Suppose that a and b are constants. If both $f(x, t)$ and $\partial f/\partial t$ are continuous in the rectangle $[a, b] \times [c, d]$, then

$$\frac{d}{dt}\int_a^b f(x, t)dx = \int_a^b \frac{\partial f}{\partial t}(x, t)dx$$

for $t \in [c, d]$.

Thm 2 Let $f(x, t)$ and $\partial f/\partial t(x, t)$ be continuous functions in $(-\infty, \infty) \times (c, d)$. Assume that the integrals $\int_{-\infty}^{\infty} |f(x, t)|dx$ and $\int_{-\infty}^{\infty} |\partial f/\partial t|dx$ converge unifromly (as improper integrals) for $t \in (c, d)$. Then

$$\frac{d}{dt}\int_{-\infty}^{\infty} f(x, t)dx = \int_{-\infty}^{\infty} \frac{\partial f}{\partial t}(x, t)dx$$

for $t \in (c, d)$.

Thm 3 If $I(t)$ is defined by $I(t) = \int_{a(t)}^{b(t)} f(x, t)dx$, where $f(x, t)$ and $\partial f/\partial t$ are continuous on the rectangle $[A, B] \times [c, d]$, where $[A, B]$ contains the unions of all intervals $[a(t), b(t)]$, and if $a(t)$ and $b(t)$ is differentiable on $[c, d]$, then

$$\frac{dI}{dt} = \int_{a(t)}^{b(t)} \frac{\partial f}{\partial t} f(x, t)dx + f(b(t), t)b'(t) - f(a(t), t)a'(t)$$

Remark: For the two or three variables we have the similar theorems.

3.ODE

First order ODE: $\frac{dy}{dt} = f(t, y)$.

First order linear equation:

$$\frac{dy}{dt} + p(t)y = q(t)$$

where $p(t)$ and $q(t)$ are given functions. By multiplying both sides of the equation with an integrating factor $\mu(x) = e^{\int p(t)dt}$, we arrive

$$\frac{d}{dt}[\mu(t)y] = q(t)\mu(t)$$

thus the general solution is

$$y = e^{-\int p(t)dt}\{\int q(t)e^{\int p(t)dt} + C\}.$$

where C is an arbitrary constant.

Seperable Equations:

$$M(x)dx + N(y)dy = 0$$

where $M(x)$ and $N(y)$ are given functions. Let H_1 and H_2 are the antiderivatives of M and N respectively. Rewrite the equation as

$$H_1'(x) + H_2'(y)\frac{dy}{dx} = 0$$

Thus the general solution is

$$H_1(x) + H_2(y) = C$$

where C is an arbitrary constant.

Exact Equations:

$$M(x, y) + N(x, y)y' = 0$$

where $M(x, y)$ and $N(x, y)$ are given functions.
If the equation is exact, $M_y = N_x$, that is, there exists a function $\psi(x, y)$ such that

$$\frac{\partial \psi}{\partial x}(x, y) = M(x, y), \frac{\partial \psi}{\partial y}(x, y) = N(x, y)$$

and such that $\psi(x, y) = C$ defines $y = \phi(x)$ implicitly as a differentiation function of x, thus the above ODE turns to $\frac{d}{dx}\psi(x, \phi(x)) = 0$, hence the general solution is $\psi(x, y) = C$ where C is an arbitrary constant.
If the equation is not exact, multiply the equation by an undetermined integrating factors $\mu(x, y)$ such that $\mu(x, y)M(x, y) + \mu(x, y)N(x, y)y' = 0$ is exact, i.e, $(\mu M)_y = (\mu N)_x$, and then solve the exact equation to get the general solution.

4.Schrodinger Equation (Example 7 on P17)

Consider the Hydrogem Atom. This is an electron moving around a proton. Let m be the mass of the electron, e the charge, and h Planck's constant divided by 2π. Let the origin of coordinates (x, y, z) be the position of the proton and let $r = (x^2 + y^2 + z^2)^{\frac{1}{2}}$ be the spherial coordinate.

Let $u(x, y, z, t)$ be the wave function which represents a possible state of the electron, and $|u|^2$ represents the probability density of the electron at position (x, y, z) and time t. If D is any region of the space, then $\iiint_D |u|^2 dxdydz$ is the probability of finding the electron in the region D at time t. Thus

$$\iiint_{\mathbb{R}^n} |u|^2 dxdydz = 1$$

The motion of the electron satisfies Schrodinger equation:

$$-ihu_t = \frac{h^2}{2m}\triangle u + \frac{e^2}{r}u$$

in all of space $-\infty < x, y, z < \infty$

Remark:

1. The coefficient $\frac{e^2}{r}$ is called the potential. For any other atom with a single electron, e^2 is replaced by Ze^2, where Z is the atomic number.

2. With many particles (electrons), the wave function u is a function of a large number of variables. The Shrodinger Equation then becomes:

$$-ihu_t = \sum_{n=1}^{n} \frac{h^2}{2m_i}(u_{x_i x_i} + u_{y_i y_i} + u_{z_i z_i}) + V(x_1, \cdots, z_n)u$$

where the potential V depends onf all the $3n$ coordinates.

3. If we use the operator A to denote the observable quantities, then the expected value of the observable A equals

$$\iiint_D Au(x, y, z, t) \cdot \overline{u}(x, y, z, t) dxdydz$$

For example, the position is given by the operator $Au = xu$, and the momentum is given by $Au = -ih\nabla u$.