QUANTUM CHEMISTRY

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QC-1.2-FUNCTIONS

I. REAL AND COMPLEX FUNCTIONS.

Ψ_1 = Asinx (Real)

Ψ_2 = iAsinx (Imaginary)

Ψ_3 = Asinx+iAsinx (Complex)

Ψ_4 = -iAsinx (Complex conjugate of Ψ_2) = Ψ_2^*

Ψ_2 & Ψ_4 are complex conjugate to each other

Ψ_5 = Asinx-iAsinx (Complex conjugate of Ψ_3) = Ψ_3^*

Ψ_3 & Ψ_5 are complex conjugate to each other

$\Psi_1 = \Psi_1^*$(Ψ_1 is real)

NB:

$\Psi = \Psi^*$(Ψ is real)

$\Psi\Psi^*$(is real)

$z = r(\cos\theta + i\sin\theta)$

$z^n = r^n e^{in\theta} = r^n(\cos\theta + i\sin\theta)^n$

$= r^n (\cos n\theta + i\sin n\theta)$: ***Demoviour*** theorem.

Linear combinations

Ψ_6 = Asinx + iBsinx (Complex)

Ψ_7 = Asinx + iBcosx (Complex)

Ψ_8 = Asinx - iBsinx (Complex)

Ψ_9 = Asinx - iBcosx (Complex)

HW:

Let

Ψ_1 = Asinx ; Ψ_2 =- iAsinx

Ψ_3 = A(sinx + isinx); Ψ_4 = A(sinx-isinx)

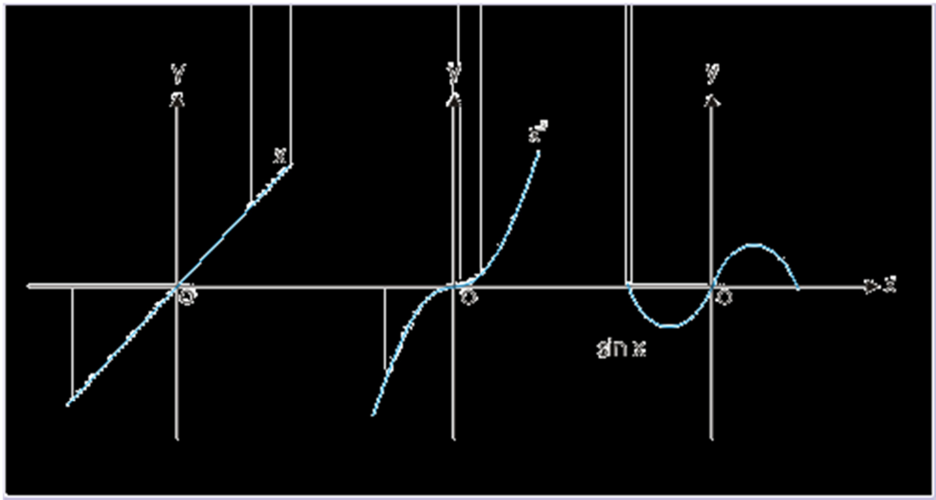
$\Psi_5 = Ae^{imx}$ = A(cosmx + isinmx) = $A(\cos x + i\sin x)^m$

$\Psi_6 = Ae^{-imx}$ = A(cosmx-isinmx) = $A(\cos x - i\sin x)^m$

Determine the following: (i) $\Psi_3\Psi_3^*$ (ii) Ψ_3^2 (iii) Ψ_6^* (iv) $\Psi_6\Psi_6^*$

II. ODD FUNCTIONS

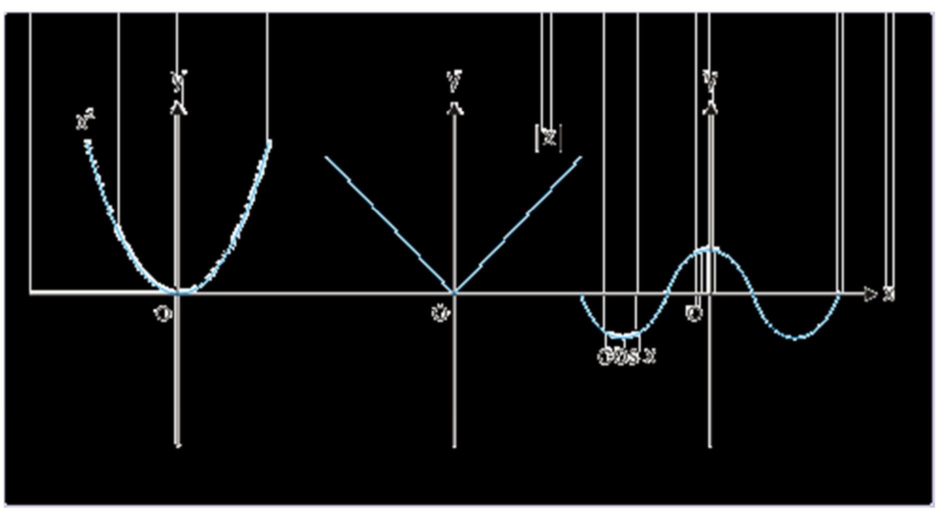
- A function f(x) is said to be "odd" if for every "x", there exists "-x" in the domain of the function such that : f(-x) = -f(x)
- Let f(x) = sinx ; f(-x) = sin(-x) = -sinx = -f(x)
- An odd function is anti symmetric about y-axis.



- **Examples:** x, x^3, sinx, sinhx, ax^2+bx ; ax^2+bx+c

III. EVEN FUNCTIONS

- A function f(x) is said to be "even" if for every "x", there exists "-x" in the domain of the function such that : f(-x) = f(x)
- Let f(x) = cosx ; f(-x) = cos(-x) = cosx = f(x)
- An even function is symmetric about y-axis.



- **Examples:** x^2, x^4, cosx, coshx, e^x+e^{-x}, ax^2 , ax^2+c

Problem 1: Prove that the function f(x) is even

$$f(x) = x\,\frac{a^x-1}{a^x+1}$$

IV. BASIC PROPERTIES OF ODD AND EVEN FUNCTIONS

- The **sum** of an even and odd function is neither even nor odd: sinx + cosx
- The sum of two even functions is even, and any constant multiple of an even function is even.
- The sum of two odd functions is odd, and any constant multiple of an odd function is odd.

  $x^4 + 2x^2 + 6$ is even

  $x^2\cos(x)$ is even

  $x^3\cos(x)$ is odd

  $5x^7 + 4\sin(x)$ is odd
- The **product** of two even functions is an even function.
- The product of two odd functions is an even function.
- The product of an even function and an odd function is an odd function.
- The **quotient** of two even functions is an even function.
- The quotient of two odd functions is an even function.
- The quotient of an even function and an odd function is an odd function.

f(x)	g(x)	f(x) ± g(x)	f(x)g(x)	f(x)/g(x)
Odd	odd	odd	even	even
odd	even	neither	odd	odd
even	even	even	even	even

While some functions are ***neither*** even *nor* odd

$$x^4 + 6x + 1\ ;\ \cos(x) + x^5;\ x^3 + 1\ ;\ \ln(x)\ ;\ a^x\ ;\ e^{-imx}\ ;\ e^{imx}$$

- The **derivative** of an even function is odd.
- The derivative of an odd function is even.

- The **integral** of an odd function from −*A* to +*A* is zero .
- The integral of an even function from −*A* to +*A* is twice the integral from 0 to +*A*(Half interval).
- Determine each function given below as **even, odd** or **neither**.

1. $x^4 + 6x^2 + 1$
2. $x\cos(x) + x^3$; xsinx
3. 1/x
4. 3x + 9
5. $\sin(x^2)$; $\sin^2 x$; $\sin(x^2)$; $\sin^2 x^2$
6. $x^3 + 1$
7. $\sin^3(x)$
8. $\sin^2(x^2) + x^2 + 1$

V. CLOSED INTERVAL is an interval that includes the extreme limits : **$a \le x \le b$.**

VI. OPEN INTERVAL is an interval that does not include the extreme limits :

$a < x < b$

VII. ORTHOGONALFUNCTIONS

Two functions ψ_1& ψ_2 are said to be orthogonal in the range $a \le x \le b$ if the integral$\int \psi_1\psi_2 dx = 0$ in the range $a \le x \le b$.

Examples: Asin(nx), Bcos(nx) for integral values of n.

VIII. NORMALIZED FUNCTIONS

A function ψ is said to be normalized in the range $a \le x \le b$ if the integral $\int \psi\psi^* dx = 1$ in the range $a \le x \le b$.

- Normalize $(-x^2/2)$ & Ax^2 in the range (-a, +a)
- Normalize Asinx & Bcosx for $0 \le x \le \pi/2$
- Normalize Asinx & Bcosx in the range $(0, \pi)$
- Normalize Ae^x in the range (0, 1)

IX. ORTHONORMAL SET OF FUNCTIONS

A set of function,in a given range of limits, such that each one is normalized and orthogonal to each other

Examples:

- $(2/l)^{1/2}\sin(n\pi x/l)$, for integral values of n and for $0 \le x \le l$.

- $(1/2\pi)^{1/2} e^{-imx}$ for integral values of m and for $0 \leq x \leq 2\pi$

X. WELBEHAVED WAVE FUNCTIONS (Acceptable wave function)

Single valued, Continuous, Normalized, Orthogonal & should disappear at the extreme limits

XI. DIFFERENTIALEQUATIONS

$$\frac{dy}{dx} = Ax + k \qquad \text{OR} \; dy = (Ax + k)\, dx$$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0 \qquad \text{order: 2 ; degree: 1}$$

XII. ORDER AND DEGREE.

Order: The number of the highest derivative in a differential equation.

$$\frac{dy}{dx} = Ax + k \qquad \text{order: 1 ; degree: 1}$$

$$\frac{d^2y}{dx^2} = Ax + k \qquad \text{order: 2 ; degree: 1}$$

$$\left\{\frac{dy}{dx}\right\}^2 = Ax + k \qquad \text{order: 1 ; degree: 2}$$

$$\left\{\frac{d^2y}{dx^2}\right\} = Ax + k \qquad \text{order: 2 ; degree: 1}$$

$$\left\{\frac{d^2y}{dx^2}\right\}^2 + \frac{dy}{dx} = Ax + k$$ order: 2 ; degree: 2

$$\left\{\frac{d^2y}{dx^2}\right\} + \left\{\frac{dy}{dx}\right\}^2 = Ax + k$$ order: 2 ; degree: 1

$$\left(\frac{d^2y}{dx^2}\right)^3 + \frac{dy}{dx} = \sin x$$ order 2 and degree 3.

$$\frac{d^3y}{dx^3} + 4x\left(\frac{dy}{dx}\right)^2 = y\frac{d^2y}{dx^2} + e^y$$ order 3 drgree 1

XIII. SOLUTIONS TO TYPICAL DIFFERENTIAL EQUATIONS.

$$\frac{dy}{dx} = Ax + k$$

$$dy = (Ax + k)\, dx$$

Hence, the function y can obtain by integration.