Chemistry 4507 - Physical Chemistry I

Lecture Handout - **Useful Formulae**

Laplacian Operators:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}$$

Common Integrals:

$$\int kx^n \, dx = k\frac{x^{n+1}}{(n+1)} + const, \text{ for all } n \neq -1$$

$$\int k\frac{1}{x} dx = k\ln(x) + const = \ln(x^k) + const$$

$$\int e^{kx} \, dx = \frac{1}{k}e^{kx} + const$$

$$\int \sin(kx)\, dx = -\frac{1}{k}\cos(kx) + const$$

$$\int \cos(kx)\, dx = +\frac{1}{k}\sin(kx) + const$$

$$\int \cos(kx)\sin(kx)\, dx = \frac{1}{2k}\cos^2(kx) + const$$

$$\int_{-a}^{+a} f_{even}(x)\, dx = 2\int_{0}^{+a} f_{even}(x)\, dx$$

$$\int_{-a}^{+a} f_{odd}(x)\, dx = 0$$

Gaussian Integrals:

$$\int_{-\infty}^{+\infty} x^{2n} e^{-ax^2}\, dx = 2\int_{0}^{+\infty} x^{2n} e^{-ax^2}\, dx = \frac{(2n)!\sqrt{\pi}}{n! 2^{2n} a^{(2n+1)/2}} = (-1)^n \frac{d^n}{da^n}\left(\int_{-\infty}^{+\infty} e^{-ax^2}\, dx\right) = (-1)^n \frac{d^n}{da^n}\left(\sqrt{\frac{\pi}{a}}\right)$$

$$\int_{0}^{+\infty} x^{2n+1} e^{-ax^2}\, dx = -\int_{-\infty}^{0} x^{2n+1} e^{-ax^2}\, dx = \frac{n!}{2a^{(n+1)}}$$

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Taylor Series Expansion:

$$F(z)=\sum_{k=0}^{\infty}\frac{1}{k!}\left[\frac{d^k}{dz^k}F(z=z_0)\right](z-z_0)^k=\frac{F(z_0)}{0!}+\frac{F'(z_0)}{1!}(z-z_0)+\frac{F''(z_0)}{2!}(z-z_0)^2+\frac{F'''(z_0)}{3!}(z-z_0)^3+\ldots$$

Trigonometric Identities:

$\cos(\beta)=\cos(-\beta)$ EVEN FUNCTION	$\sin(-\beta)=-\sin(\beta)$ ODD FUNCTION
$\cos(\alpha+\beta)=\cos(\alpha)\cos(\beta)-\sin(\alpha)\sin(\beta)$	$\sin(a+\beta)=\sin(\alpha)\cos(\beta)+\sin(\beta)\cos(\alpha)$
$\cos(2\alpha)=\cos^2(\alpha)-\sin^2(\alpha)$	$\sin(2\alpha)=2\sin(\alpha)\cos(\alpha)$
$\cos(\alpha-\beta)=\cos(\alpha)\cos(\beta)+\sin(\alpha)\sin(\beta)$	$\sin(a-\beta)=\sin(\alpha)\cos(\beta)-\sin(\beta)\cos(\alpha)$
$\cos(0)=1=\cos^2(\alpha)+\sin^2(\alpha)$	

Rudimentary Linear Algebra:

$$\det(\mathbf{A})=|\mathbf{A}|=\det\begin{pmatrix}a_{11}&a_{12}&a_{13}\\a_{21}&a_{22}&a_{23}\\a_{31}&a_{32}&a_{33}\end{pmatrix}$$

$$=a_{11}\det\begin{pmatrix}a_{22}&a_{23}\\a_{32}&a_{33}\end{pmatrix}-a_{12}\det\begin{pmatrix}a_{21}&a_{23}\\a_{31}&a_{33}\end{pmatrix}+a_{13}\det\begin{pmatrix}a_{21}&a_{22}\\a_{31}&a_{32}\end{pmatrix}$$

$$=a_{11}\left[a_{22}a_{33}-a_{23}a_{32}\right]-a_{12}\left[a_{21}a_{33}-a_{23}a_{31}\right]+a_{13}\left[a_{21}a_{32}-a_{22}a_{31}\right]$$

Rudimentary Complex Algebra:

$$i=\sqrt{-1}$$

$$z=(x+iy)=r(\cos\theta+i\sin\theta)=re^{i\theta}$$

$$z^*=(x-iy)=r(\cos\theta-i\sin\theta)=re^{-i\theta}$$

$$|z|=\left(z^*\cdot z\right)^{1/2}=\left(x^2+y^2\right)^{1/2}=\left(re^{-i\theta}\cdot re^{+i\theta}\right)^{1/2}=\left(r^2e^{-i\theta+i\theta}\right)^{1/2}=r$$