Mathematical Handbook for Elementary Quantum Mechanics

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Contents

1 Pure Mathematics

Here are some fundamental maths[1] that are often used in quantum mechanics. Certainly, you might have met them in high school, anyway they are gathered and listed below.

1.1 Trigonometry

1. Basic trigonometric formulas:

$$\sin(\alpha+\beta) = \sin\alpha\cos\beta + \cos\alpha\sin\beta, \tag{1.1}$$
$$\sin(\alpha-\beta) = \sin\alpha\cos\beta - \cos\alpha\sin\beta, \tag{1.2}$$
$$\cos(\alpha+\beta) = \cos\alpha\cos\beta - \sin\alpha\sin\beta, \tag{1.3}$$
$$\cos(\alpha-\beta) = \cos\alpha\cos\beta + \sin\alpha\sin\beta. \tag{1.4}$$

2. Prosthaphaeresis:

$$\sin\alpha\sin\beta = \frac{\cos(\alpha-\beta)-\cos(\alpha+\beta)}{2}, \tag{1.5}$$
$$\cos\alpha\cos\beta = \frac{\cos(\alpha-\beta)+\cos(\alpha+\beta)}{2}, \tag{1.6}$$
$$\sin\alpha\cos\beta = \frac{\sin(\alpha+\beta)+\sin(\alpha-\beta)}{2}, \tag{1.7}$$
$$\cos\alpha\sin\beta = \frac{\sin(\alpha+\beta)-\sin(\alpha-\beta)}{2}. \tag{1.8}$$

Reverse identities of prosthaphaeresis:

$$\sin\alpha+\sin\beta = 2\sin\left(\frac{\alpha+\beta}{2}\right)\cos\left(\frac{\alpha-\beta}{2}\right), \tag{1.9}$$
$$\sin\alpha-\sin\beta = 2\cos\left(\frac{\alpha+\beta}{2}\right)\sin\left(\frac{\alpha-\beta}{2}\right), \tag{1.10}$$
$$\cos\alpha+\cos\beta = 2\cos\left(\frac{\alpha+\beta}{2}\right)\cos\left(\frac{\alpha-\beta}{2}\right), \tag{1.11}$$
$$\cos\alpha-\cos\beta = -2\sin\left(\frac{\alpha+\beta}{2}\right)\sin\left(\frac{\alpha-\beta}{2}\right). \tag{1.12}$$

3. Law of cosines: if $\boldsymbol{c} = \boldsymbol{a} + \boldsymbol{b}$, then[2]

$$c^2 = a^2 + b^2 + 2ab\cos\theta, \quad \text{or} \quad \boldsymbol{a}\cdot\boldsymbol{b} = \frac{1}{2}\left(c^2 - a^2 - b^2\right). \tag{1.13}$$

4. Half-angle formula:

$$\sin\frac{\alpha}{2} = \pm\sqrt{\frac{1-\cos\alpha}{2}}, \tag{1.14}$$
$$\cos\frac{\alpha}{2} = \pm\sqrt{\frac{1+\cos\alpha}{2}}, \tag{1.15}$$
$$\tan\frac{\alpha}{2} = \pm\sqrt{\frac{1-\cos\alpha}{1+\cos\alpha}} = \frac{1-\cos\alpha}{\sin\alpha} = \frac{\sin\alpha}{1+\cos\alpha}, \tag{1.16}$$
$$\cot\frac{\alpha}{2} = \pm\sqrt{\frac{1+\cos\alpha}{1-\cos\alpha}} = \frac{1+\cos\alpha}{\sin\alpha} = \frac{\sin\alpha}{1-\cos\alpha}. \tag{1.17}$$

[1] For further maths, see *Qiu, G.W. Notes on Mathematical Methods for Physics II (Second Edition). April 2017.*

[2] The second form usually appears for angular momentum, e.g. $\boldsymbol{J} \equiv \boldsymbol{L} + \boldsymbol{S}, \quad \Rightarrow \quad \boldsymbol{L}\cdot\boldsymbol{S} = \frac{1}{2}\left(J^2 - L^2 - S^2\right)$.
The trick also goes for three or more vectors:

$$\boldsymbol{S} \equiv \boldsymbol{S}_1 + \boldsymbol{S}_2 + \boldsymbol{S}_3, \quad \Rightarrow \quad \boldsymbol{S}_1\cdot\boldsymbol{S}_2 + \boldsymbol{S}_2\cdot\boldsymbol{S}_3 + \boldsymbol{S}_3\cdot\boldsymbol{S}_1 = \frac{1}{2}\left(S^2 - S_1^2 - S_2^2 - S_3^2\right).$$

Moreover, we have $|\boldsymbol{r}_1 - \boldsymbol{r}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos\theta_{12}}$, which is also very useful.

5. Duplication formula:

$$\sin(2\alpha) = 2\cos\alpha\sin\alpha, \tag{1.18}$$
$$\cos(2\alpha) = \cos^2\alpha - \sin^2\alpha = 2\cos^2\alpha - 1 = 1 - 2\sin^2\alpha, \tag{1.19}$$
$$\sin(3\alpha) = 3\cos^2\alpha\sin\alpha - \sin^3\alpha = 3\sin\alpha - 4\sin^3\alpha, \tag{1.20}$$
$$\cos(3\alpha) = \cos^3\alpha - 3\cos\alpha\sin^2\alpha = 4\cos^3\alpha - 3\cos\alpha. \tag{1.21}$$

Generalization[3]:

$$\begin{aligned}\sin(n\alpha) &= \sum_{k=1,3,5,\cdots} (-1)^{\frac{k-1}{2}} \binom{n}{k} \cos^{n-k}\alpha\sin^k\alpha \\ &= n\cos^{n-1}\alpha\sin\alpha - \binom{n}{3}\cos^{n-3}\alpha\sin^3\alpha + \binom{n}{5}\cos^{n-5}\alpha\sin^5\alpha - \cdots;\end{aligned} \tag{1.22}$$

$$\begin{aligned}\cos(n\alpha) &= \sum_{k=0,2,4,\cdots} (-1)^{\frac{k}{2}} \binom{n}{k} \cos^{n-k}\alpha\sin^k\alpha \\ &= \cos^n\alpha - \binom{n}{2}\cos^{n-2}\alpha\sin^2\alpha + \binom{n}{4}\cos^{n-4}\alpha\sin^4\alpha - \cdots.\end{aligned} \tag{1.23}$$

6. Powers of trigonometric functions:

$$\sin^2\alpha = \frac{1}{2}(-\cos 2\alpha + 1), \tag{1.24}$$
$$\cos^2\alpha = \frac{1}{2}(\cos 2\alpha + 1), \tag{1.25}$$
$$\sin^3\alpha = \frac{1}{4}(-\sin 3\alpha + 3\sin\alpha), \tag{1.26}$$
$$\cos^3\alpha = \frac{1}{4}(\cos 3\alpha + 3\cos\alpha). \tag{1.27}$$

Generalization:

$$\sin^{2n}\alpha = \frac{1}{2^{2n}}\left\{\sum_{k=0}^{n-1}(-1)^{n-k}2\binom{2n}{k}\cos[2(n-k)\alpha] + \binom{2n}{n}\right\}, \tag{1.28}$$
$$\cos^{2n}\alpha = \frac{1}{2^{2n}}\left\{\sum_{k=0}^{n-1}2\binom{2n}{k}\cos[2(n-k)\alpha] + \binom{2n}{n}\right\}, \tag{1.29}$$
$$\sin^{2n-1}\alpha = \frac{1}{2^{2n-2}}\sum_{k=0}^{n-1}(-1)^{n+k-1}\binom{2n-1}{k}\sin[(2n-2k-1)\alpha], \tag{1.30}$$
$$\cos^{2n-1}\alpha = \frac{1}{2^{2n-2}}\sum_{k=0}^{n-1}\binom{2n-1}{k}\cos[(2n-2k-1)\alpha]. \tag{1.31}$$

1.2 Series

1. Geometric series:

$$\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n = 1 + x + x^2 + x^3 + \cdots \qquad (|x| < 1), \tag{1.32}$$
$$\frac{1}{(1-x)^2} = \sum_{n=1}^{\infty} nx^{n-1} = 1 + 2x + 3x^2 + 4x^3 + \cdots \qquad (|x| < 1), \tag{1.33}$$
$$\frac{1}{(1-x)^3} = \sum_{n=2}^{\infty} \frac{n(n-1)}{2}x^{n-2} = 1 + 3x + 6x^2 + 10x^3 + \cdots \qquad (|x| < 1). \tag{1.34}$$

[3]Derived from de Moivre's identity $(\cos\alpha + \mathrm{i}\sin\alpha)^n = \cos(n\alpha) + \mathrm{i}\sin(n\alpha)$.

2. Power series:

$$f(x)=\sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}x^n=f(0)+xf'(0)+\frac{x^2}{2!}f''(0)+\frac{x^3}{3!}f'''(0)+\cdots, \tag{1.35}$$

$$\mathrm{e}^x=\sum_{n=0}^{\infty}\frac{x^n}{n!}=1+x+\frac{x^2}{2!}+\frac{x^3}{3!}+\cdots, \tag{1.36}$$

$$\sin x=\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)!}x^{2n+1}=x-\frac{x^3}{3!}+\frac{x^5}{5!}-\frac{x^7}{7!}+\cdots, \tag{1.37}$$

$$\cos x=\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n)!}x^{2n}=1-\frac{x^2}{2!}+\frac{x^4}{4!}-\frac{x^6}{6!}+\cdots, \tag{1.38}$$

$$\sinh x=\sum_{n=0}^{\infty}\frac{x^{2n+1}}{(2n+1)!}=x+\frac{x^3}{3!}+\frac{x^5}{5!}+\frac{x^7}{7!}+\cdots, \tag{1.39}$$

$$\cosh x=\sum_{n=0}^{\infty}\frac{x^{2n}}{(2n)!}=1+\frac{x^2}{2!}+\frac{x^4}{4!}+\frac{x^6}{6!}+\cdots, \tag{1.40}$$

$$(1+x)^m=\sum_{n=0}^{\infty}\frac{\Gamma(a+1)}{\Gamma(a-n+1)}\frac{x^n}{n!}=1+ax+\frac{a(a-1)}{2!}x^2+\frac{a(a-1)(a-2)}{3!}x^3+\cdots, \tag{1.41}$$

$$\ln(1+x)=\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}x^n=x-\frac{x^2}{2}+\frac{x^3}{3}-\frac{x^4}{4}+\cdots. \tag{1.42}$$

3. Some special series:

$$\sum_{n=1}^{\infty}\frac{1}{n^2}=\frac{1}{1^2}+\frac{1}{2^2}+\frac{1}{3^2}+\frac{1}{4^2}\cdots=\frac{\pi^2}{6}, \tag{1.43}$$

$$\sum_{n=1}^{\infty}\frac{1}{n^4}=\frac{1}{1^4}+\frac{1}{2^4}+\frac{1}{3^4}+\frac{1}{4^4}\cdots=\frac{\pi^4}{90}, \tag{1.44}$$

$$\sum_{n=1}^{\infty}\frac{1}{n^6}=\frac{1}{1^6}+\frac{1}{2^6}+\frac{1}{3^6}+\frac{1}{4^6}\cdots=\frac{\pi^6}{945}, \tag{1.45}$$

$$\sum_{n=1,3,5,\cdots}\frac{1}{n^2}=\frac{1}{1^2}+\frac{1}{3^2}+\frac{1}{5^2}+\frac{1}{7^2}\cdots=\frac{\pi^2}{8}, \tag{1.46}$$

$$\sum_{n=1,3,5,\cdots}\frac{1}{n^4}=\frac{1}{1^4}+\frac{1}{3^4}+\frac{1}{5^4}+\frac{1}{7^4}\cdots=\frac{\pi^4}{96}, \tag{1.47}$$

$$\sum_{n=1,3,5,\cdots}\frac{1}{n^6}=\frac{1}{1^6}+\frac{1}{3^6}+\frac{1}{5^6}+\frac{1}{7^6}\cdots=\frac{\pi^6}{960}. \tag{1.48}$$

4. Multiplication of power series:

$$\sum_{n=0}^{\infty}a_nx^n\sum_{n=0}^{\infty}b_nx^n=\sum_{n=0}^{\infty}\sum_{m=0}^{n}a_mb_{n-m}x^n. \tag{1.49}$$

1.3 Integrals

1.3.1 Definite Integrals

1. Integral by parts:

$$\int_a^b \mu\nu'\,\mathrm{d}x=\mu\nu\Big|_a^b-\int_a^b\mu'\nu\,\mathrm{d}x. \tag{1.50}$$

2. Exponential integrals:

$$\int_0^{\infty}x^n\mathrm{e}^{-x/a}\,\mathrm{d}x=n!\,a^{n+1}. \tag{1.51}$$

First few: (Often used in Hydrogen atom)

$$\int_0^\infty x\mathrm{e}^{-x/a}\,\mathrm{d}x = a^2, \tag{1.52}$$

$$\int_0^\infty x^2\mathrm{e}^{-x/a}\,\mathrm{d}x = 2a^3, \tag{1.53}$$

$$\int_0^\infty x^3\mathrm{e}^{-x/a}\,\mathrm{d}x = 6a^4, \tag{1.54}$$

$$\int_0^\infty x^4\mathrm{e}^{-x/a}\,\mathrm{d}x = 24a^5, \tag{1.55}$$

$$\int_0^\infty x^5\mathrm{e}^{-x/a}\,\mathrm{d}x = 120a^6. \tag{1.56}$$

3. Gaussian integrals:

$$\int_0^\infty \mathrm{e}^{-x^2/a^2}\,\mathrm{d}x = \sqrt{\pi}\left(\frac{a}{2}\right), \tag{1.57}$$

$$\int_0^\infty x^{2n}\mathrm{e}^{-x^2/a^2}\,\mathrm{d}x = \sqrt{\pi}\frac{(2n)!}{n!}\left(\frac{a}{2}\right)^{2n+1}, \tag{1.58}$$

$$\int_0^\infty x^{2n+1}\mathrm{e}^{-x^2/a^2}\,\mathrm{d}x = \frac{n!}{2}a^{2n+2}. \tag{1.59}$$

First few: (Often used in Hydrogen atom[4])

$$\int_0^\infty x\mathrm{e}^{-x^2/a^2}\,\mathrm{d}x = \frac{1}{2}a^2, \tag{1.60}$$

$$\int_0^\infty x^2\mathrm{e}^{-x^2/a^2}\,\mathrm{d}x = \frac{\sqrt{\pi}}{4}a^3, \tag{1.61}$$

$$\int_0^\infty x^3\mathrm{e}^{-x^2/a^2}\,\mathrm{d}x = \frac{1}{2}a^4, \tag{1.62}$$

$$\int_0^\infty x^4\mathrm{e}^{-x^2/a^2}\,\mathrm{d}x = \frac{3\sqrt{\pi}}{8}a^5, \tag{1.63}$$

$$\int_0^\infty x^5\mathrm{e}^{-x^2/a^2}\,\mathrm{d}x = a^6. \tag{1.64}$$

Alternative form:

$$\int_{-\infty}^\infty \mathrm{e}^{-ax^2+bx}\,\mathrm{d}x = \sqrt{\frac{\pi}{a}}\mathrm{e}^{b^2/4a}. \tag{1.65}$$

4. Wallis' integrals:

$$I_{2n} = \int_0^{\pi/2}\sin^{2n}x\,\mathrm{d}x = \int_0^{\pi/2}\cos^{2n}x\,\mathrm{d}x = \frac{(2n-1)!!}{(2n)!!}\frac{\pi}{2}, \tag{1.66}$$

$$I_{2n+1} = \int_0^{\pi/2}\sin^{2n+1}x\,\mathrm{d}x = \int_0^{\pi/2}\cos^{2n+1}x\,\mathrm{d}x = \frac{(2n)!!}{(2n+1)!!}. \tag{1.67}$$

5. An integral concerning delta function:

$$\int_{-\alpha}^{\alpha}\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k = \frac{\mathrm{e}^{\mathrm{i}\alpha x}-\mathrm{e}^{-\mathrm{i}\alpha x}}{\mathrm{i}x} = \frac{2}{x}\sin(\alpha x), \tag{1.68}$$

$$\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k = \lim_{\alpha\to\infty}\frac{2}{x}\sin(\alpha x) = 2\pi\delta(x). \tag{1.69}$$

6. Gamma function:

$$\int_0^\infty x^{s-1}\mathrm{e}^{-x}\,\mathrm{d}x = \Gamma(s). \tag{1.70}$$

[4] Also important in variational principal, where we take Gaussian trial wave function $\psi = A\mathrm{e}^{-bx^2}$, but remember to substitute b for $1/a^2$ here.

Alternative form, when $s>0$, $\lambda>0$, $m>0$[5]:

$$\boxed{\int_0^\infty x^{s-1}\mathrm{e}^{-\lambda x^m}\,\mathrm{d}x=\frac{1}{m}\lambda^{-s/m}\Gamma\left(\frac{s}{m}\right).} \tag{1.71}$$

Euler-Riemann(Gamma-Zeta) integral:

$$\int_0^\infty \frac{x^{s-1}}{\mathrm{e}^x-1}\,\mathrm{d}x=\Gamma(s)\zeta(s)=\sum_{n=1}^\infty\frac{1}{n^s}\Gamma(s), \tag{1.72}$$

for positive integer s,

$$\int_0^\infty x^s\mathrm{e}^{-x}\,\mathrm{d}x=s!, \tag{1.73}$$

$$\int_0^\infty \frac{x^s}{\mathrm{e}^x-1}\,\mathrm{d}x=\sum_{n=1}^\infty\frac{s!}{n^{s+1}}. \tag{1.74}$$

1.3.2 Indefinite Integrals

1. Integrals of x-power with sine[6]:

$$\int x\sin(ax)\,\mathrm{d}x=\frac{1}{a^2}\sin(ax)-\frac{x}{a}\cos(ax), \tag{1.75}$$

$$\int x^2\sin(ax)\,\mathrm{d}x=\frac{2x}{a^2}\sin(ax)-\frac{a^2x^2-2}{a^3}\cos(ax), \tag{1.76}$$

$$\int x^3\sin(ax)\,\mathrm{d}x=\frac{3(a^2x^2-2)}{a^4}\sin(ax)-\frac{x(a^2x^2-6)}{a^3}\cos(ax), \tag{1.77}$$

$$\int x^4\sin(ax)\,\mathrm{d}x=\frac{4x(a^2x^2-6)}{a^4}\sin(ax)-\frac{a^2x^2(a^2x^2-12)+24}{a^5}\cos(ax). \tag{1.78}$$

Integrals of x-power with cosine:

$$\int x\cos(ax)\,\mathrm{d}x=\frac{1}{a^2}\cos(ax)+\frac{x}{a}\sin(ax), \tag{1.79}$$

$$\int x^2\cos(ax)\,\mathrm{d}x=\frac{2x}{a^2}\cos(ax)+\frac{a^2x^2-2}{a^3}\sin(ax), \tag{1.80}$$

$$\int x^3\cos(ax)\,\mathrm{d}x=\frac{3(a^2x^2-2)}{a^4}\cos(ax)+\frac{x(a^2x^2-6)}{a^3}\sin(ax), \tag{1.81}$$

$$\int x^4\cos(ax)\,\mathrm{d}x=\frac{4x(a^2x^2-6)}{a^4}\cos(ax)+\frac{a^2x^2(a^2x^2-12)+24}{a^5}\sin(ax). \tag{1.82}$$

The recursion formula is

$$\int x^n\sin(ax)\,\mathrm{d}x=-\frac{x^n}{a}\cos(ax)+\frac{n}{a}\int x^{n-1}\cos(ax)\,\mathrm{d}x, \tag{1.83}$$

$$\int x^n\cos(ax)\,\mathrm{d}x=\frac{x^n}{a}\sin(ax)-\frac{n}{a}\int x^{n-1}\sin(ax)\,\mathrm{d}x. \tag{1.84}$$

2. Integrals of powers of sine:

$$\int \sin(ax)\,\mathrm{d}x=-\frac{\cos(ax)}{a}, \tag{1.85}$$

[5]This conclusion is so remarkable that I box it out, comparing eqs.(1.51)~(1.64). You find that those Gaussian integrals are special cases for positive integer s's, with

$$\lambda=\frac{1}{a^2},\quad m=1\text{ or }2.$$

However our eq.(1.71) performs further, so my advice is to bear this equation in mind and you will never need to "recite" eqs.(1.51)~(1.64).

[6]The author is too lazy to write the constant C here.

$$\int \sin^2(ax)\,\mathrm{d}x = -\frac{\sin(2ax)}{4a} + \frac{x}{2}, \tag{1.86}$$

$$\int \sin^3(ax)\,\mathrm{d}x = \frac{\cos(3ax)}{12a} - \frac{3\cos(ax)}{4a}, \tag{1.87}$$

$$\int \sin^4(ax)\,\mathrm{d}x = \frac{\sin(4ax)}{32a} - \frac{\sin(2ax)}{4a} + \frac{3x}{8}. \tag{1.88}$$

Integrals of powers of sine:

$$\int \cos(ax)\,\mathrm{d}x = \frac{\sin(ax)}{a}, \tag{1.89}$$

$$\int \cos^2(ax)\,\mathrm{d}x = \frac{\sin(2ax)}{4a} + \frac{x}{2}, \tag{1.90}$$

$$\int \cos^3(ax)\,\mathrm{d}x = \frac{\sin(3ax)}{12a} + \frac{3\sin(ax)}{4a}, \tag{1.91}$$

$$\int \cos^4(ax)\,\mathrm{d}x = \frac{\sin(4ax)}{32a} + \frac{\sin(2ax)}{4a} + \frac{3x}{8}. \tag{1.92}$$

3. Integrals of x-power with exponential:

$$\int x\mathrm{e}^{ax}\,\mathrm{d}x = \mathrm{e}^{ax}\left(\frac{x}{a} - \frac{1}{a^2}\right), \tag{1.93}$$

$$\int x^2\mathrm{e}^{ax}\,\mathrm{d}x = \mathrm{e}^{ax}\left(\frac{x^2}{a} - \frac{2x}{a^2} + \frac{2}{a^3}\right), \tag{1.94}$$

$$\int x^3\mathrm{e}^{ax}\,\mathrm{d}x = \mathrm{e}^{ax}\left(\frac{x^3}{a} - \frac{3x^2}{a^2} + \frac{6x}{a^3} - \frac{6}{a^4}\right), \tag{1.95}$$

$$\int x^4\mathrm{e}^{ax}\,\mathrm{d}x = \mathrm{e}^{ax}\left(\frac{x^4}{a} - \frac{4x^3}{a^2} + \frac{12x^2}{a^3} - \frac{24x}{a^4} + \frac{24}{a^5}\right). \tag{1.96}$$

4. Integrals of exponential with sine or cosine:

$$\int \mathrm{e}^{ax}\sin(bx)\,\mathrm{d}x = \frac{\mathrm{e}^{ax}[a\sin(bx) - b\cos(bx)]}{a^2+b^2}, \tag{1.97}$$

$$\int \mathrm{e}^{ax}\cos(bx)\,\mathrm{d}x = \frac{\mathrm{e}^{ax}[a\cos(bx) + b\sin(bx)]}{a^2+b^2}. \tag{1.98}$$

5. Integrals of sines with cosines:

$$\int \sin(ax+b)\sin(cx+d)\,\mathrm{d}x = \frac{\sin[(a-c)x+b-d]}{2(a-c)} - \frac{\sin[(a+c)x+b+d]}{2(a+c)}, \tag{1.99}$$

$$\int \cos(ax+b)\cos(cx+d)\,\mathrm{d}x = \frac{\sin[(a-c)x+b-d]}{2(a-c)} + \frac{\sin[(a+c)x+b+d]}{2(a+c)}, \tag{1.100}$$

$$\int \sin(ax+b)\cos(cx+d)\,\mathrm{d}x = -\frac{\cos[(a-c)x+b-d]}{2(a-c)} - \frac{\cos[(a+c)x+b+d]}{2(a+c)}, \tag{1.101}$$

$$\int \cos(ax+b)\sin(cx+d)\,\mathrm{d}x = \frac{\cos[(a-c)x+b-d]}{2(a-c)} - \frac{\cos[(a+c)x+b+d]}{2(a+c)}. \tag{1.102}$$

1.4 Dirac Delta Function

1. Definition:

$$\delta(x) = \begin{cases} \infty, & \text{for } x = 0; \\ 0, & \text{for } x \neq 0. \end{cases} \qquad s.t. \qquad \int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x = 1. \tag{1.103}$$

delta function is derivative of Heaviside function

$$\delta(x) = \frac{\mathrm{d}H(x)}{\mathrm{d}x}, \qquad \text{where} \qquad H(x) = \begin{cases} 1, & \text{for } x > 0; \\ 0, & \text{for } x < 0. \end{cases} \tag{1.104}$$

Alternative expressions

$$\delta(x) = \lim_{\alpha\to\infty} \frac{1}{\pi}\frac{\sin(\alpha x)}{x}, \tag{1.105}$$

$$\delta(x) = \lim_{\alpha\to 0^+} \frac{1}{\pi}\frac{\alpha}{x^2+\alpha^2}, \tag{1.106}$$
$$\delta(x) = \lim_{\alpha\to 0^+} \frac{1}{\alpha\sqrt{\pi}} \mathrm{e}^{-(x/\alpha)^2}. \tag{1.107}$$

2. Properties:

$$\delta(-x) = \delta(x), \tag{1.108}$$
$$\delta'(-x) = -\delta'(x), \tag{1.109}$$
$$\delta(\alpha x) = \frac{1}{|\alpha|}\delta(x), \tag{1.110}$$
$$f(x)\delta(x-\xi) = f(\xi)\delta(x-\xi), \tag{1.111}$$
$$\delta(x^2-\alpha^2) = \frac{1}{2|\alpha|}\left[\delta(x+\alpha)+\delta(x-\alpha)\right]. \tag{1.112}$$

$$\int_{-\infty}^{\infty} f(x)\delta(x-\xi)\,\mathrm{d}x = f(\xi). \tag{1.113}$$
$$\int_{x_1}^{x_2} f(x)\delta(x-\xi)\,\mathrm{d}x = \begin{cases} f(\xi), & \text{for } \xi\in[x_1,x_2]; \\ 0, & \text{otherwise.}\end{cases} \tag{1.114}$$
$$\int_{-\infty}^{\infty} \delta(\xi-x)\delta(x-\eta)\,\mathrm{d}x = \delta(\xi-\eta), \tag{1.115}$$
$$\int_{-\infty}^{\infty} f(x)\delta'(x-\xi)\,\mathrm{d}x = -f'(\xi), \tag{1.116}$$
$$\int_{-\infty}^{\infty} f(x)\frac{\mathrm{d}^n}{\mathrm{d}x^n}\delta(x-\xi)\,\mathrm{d}x = (-1)^n\left[\frac{\mathrm{d}^n}{\mathrm{d}x^n}f(x)\right]_{x=\xi}. \tag{1.117}$$

3. Fourier transform
$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}\omega. \tag{1.118}$$

4. Three-dimensional delta function
$$\delta(\boldsymbol{r}) = \delta(x)\delta(y)\delta(z). \tag{1.119}$$
$$\delta(\alpha\boldsymbol{r}) = \frac{1}{|\alpha|^3}\delta(\boldsymbol{r}). \tag{1.120}$$
$$\nabla^2\frac{1}{r} = -4\pi\delta(\boldsymbol{r}). \tag{1.121}$$

1.5 Linear Algebra

1. For matrices(operators) A, B and C, we have

$$[A,BC] = [A,B]C + B[A,C], \tag{1.122}$$
$$[AB,C] = A[B,C] + [A,C]B. \tag{1.123}$$

2. For matrices A and B, we have following identities

$$[A,B^n] = \sum_{s=0}^{n-1} B^s[A,B]B^{n-s-1}, \tag{1.124}$$
$$[A^n,B] = \sum_{s=0}^{n-1} A^s[A,B]A^{n-s-1}. \tag{1.125}$$

If matrices A and B don't commute, but both commute with $[A,B]$, we have

$$[A,B^n] = nB^{n-1}[A,B], \tag{1.126}$$
$$[A^n,B] = nA^{n-1}[A,B]. \tag{1.127}$$

Moreover, call $C = [A, B]$,

$$[A, \mathrm{e}^{\lambda B}] = \lambda C \mathrm{e}^{B}, \tag{1.128}$$

$$[A, f(B)] = C f'(B); \tag{1.129}$$

and

$$\mathrm{e}^{\lambda(A+B)} = \mathrm{e}^{\lambda A}\mathrm{e}^{\lambda B}\mathrm{e}^{-\frac{1}{2}\lambda^2 C} = \mathrm{e}^{\lambda B}\mathrm{e}^{\lambda A}\mathrm{e}^{\frac{1}{2}\lambda^2 C}. \tag{1.130}$$

3. If we have eigenfunction $Au_n = \lambda_n u_n$, then

$$\mathrm{e}^{A} u_n = \mathrm{e}^{\lambda_n} u_n, \tag{1.131}$$

$$f(A) u_n = f(\lambda_n) u_n. \tag{1.132}$$

4. For matrices A and B, let $C_0 = B$, $C_1 = [A, B]$, $C_2 = [A, C_1] = [A, [A, B]]$, $\cdots$, and λ as an constant. We have

$$\mathrm{e}^{\lambda A} B \mathrm{e}^{-\lambda A} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} C_n = B + \lambda [A, B] + \frac{\lambda^2}{2!} [A, [A, B]] + \cdots . \tag{1.133}$$

2 Physics

I'm not actually talking about physics in this section, but some tricks in maths that you are welcome to bear in mind.

2.1 Harmonic Oscillator

The Schrödinger equation for harmonic oscillator says

$$\frac{1}{2m}\left[p^2+(m\omega x)^2\right]\psi=E\psi. \tag{2.1}$$

Let

$$a_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp \mathrm{i}p+m\omega x), \tag{2.2}$$

then

$$[a_-,a_+]=1,\quad H=\hbar\omega\left(a_\pm a_\mp \pm\frac{1}{2}\right), \tag{2.3}$$

$$x=\sqrt{\frac{\hbar}{2m\omega}}(a_++a_-),\quad p=\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}(a_+-a_-). \tag{2.4}$$

And the eigenstates and energies are

$$\psi_0(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\mathrm{e}^{-\frac{m\omega}{2\hbar}x^2},\quad \psi_n(x)=\frac{1}{\sqrt{n}}(a_+)^n\psi_0,\quad E_n=\left(n+\frac{1}{2}\right)\hbar\omega. \tag{2.5}$$

Call the nth state $|n\rangle$, then something useful is

$$\boxed{a_+|n\rangle=\sqrt{n+1}|n+1\rangle,\quad a_-|n\rangle=\sqrt{n}|n-1\rangle.} \tag{2.6}$$

With eqs.(2.4) and (2.6), we have

$$\begin{aligned}\langle m|x|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle m|(a_++a_-)|n\rangle=\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\langle m|n+1\rangle+\sqrt{n}\langle m|n-1\rangle\right)\\ &=\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\delta_{m,n+1}+\sqrt{n}\delta_{m,n-1}\right), \end{aligned}\tag{2.7}$$

$$\begin{aligned}\langle m|x^2|n\rangle &= \frac{\hbar}{2m\omega}\langle m|(a_+^2+a_+a_-+a_-a_++a_-^2)|n\rangle\\ &=\frac{\hbar}{2m\omega}\left(\sqrt{n+1}\langle m|a_+|n+1\rangle+\sqrt{n}\langle m|a_+|n-1\rangle+\sqrt{n+1}\langle m|a_-|n+1\rangle+\sqrt{n}\langle m|a_-|n-1\rangle\right)\\ &=\frac{\hbar}{2m\omega}\left[\sqrt{(n+1)(n+2)}\delta_{m,n+2}+n\delta_{m,n}+(n+1)\delta_{m,n}+\sqrt{n(n-1)}\delta_{m,n-2}\right]. \end{aligned}\tag{2.8}$$

Similarly

$$\langle m|p|n\rangle=\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\langle m|(a_+-a_-)|n\rangle=\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\left(\sqrt{n+1}\delta_{m,n+1}-\sqrt{n}\delta_{m,n-1}\right), \tag{2.9}$$

$$\begin{aligned}\langle m|p^2|n\rangle &= -\frac{\hbar m\omega}{2}\langle m|(a_+^2-a_+a_--a_-a_++a_-^2)|n\rangle\\ &=-\frac{\hbar m\omega}{2}\left[\sqrt{(n+1)(n+2)}\delta_{m,n+2}-n\delta_{m,n}-(n+1)\delta_{m,n}+\sqrt{n(n-1)}\delta_{m,n-2}\right]. \end{aligned}\tag{2.10}$$

You may work out by yourself $\langle m|x^k|n\rangle$ or $\langle m|p^k|n\rangle$, for $k\geq 3$. Anyway, eqs.(2.7)∼(2.10) are most commonly used in perturbation theory for harmonic oscillators.

2.2 Hydrogen Atom

This is three-dimensional quantum mechanics, the Shcrödinger equation says

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\right)\psi=E\psi, \tag{2.11}$$

where

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{2.12}$$

The angular part is described by spherical harmonics Y_l^m, define angular momentum operators

$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right], \quad L_z = -\mathrm{i}\hbar\frac{\partial}{\partial\phi}, \tag{2.13}$$

then

$$\boxed{L^2 Y_l^m = \hbar^2 l(l+1) Y_l^m, \quad L_z Y_l^m = \hbar m Y_l^m.} \tag{2.14}$$

And our wave function carries Y_l^m, so

$$\frac{1}{2m_e r^2}\left[-\hbar^2\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + L^2\right]\psi - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\psi = E\psi. \tag{2.15}$$

The final solution to the Hydrogen wave function is

$$\psi_{nlm}(r,\theta,\phi) = \sqrt{\left(\frac{2}{na}\right)^2\frac{(n-l-1)!}{2n(n+l)!}}\mathrm{e}^{-r/na}\left(\frac{2r}{na}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)Y_l^m(\theta,\phi), \tag{2.16}$$

where a is so-called Bohr radius. Note that

$$a \equiv \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = 0.529\text{Å}, \quad E_n = -\left[\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{-13.6\,\mathrm{eV}}{n^2}. \tag{2.17}$$

One important equation is named Kramer's relation

$$\frac{s+1}{n^2}\langle r^s\rangle - (2s+1)a\langle r^{s-1}\rangle + \frac{s}{4}\left[(2l+1)^2 - s^2\right]a^2\langle r^{s-2}\rangle = 0. \tag{2.18}$$

With this relation, we have

$$\boxed{\left\langle\frac{1}{r}\right\rangle = \frac{1}{n^2 a}, \quad \left\langle\frac{1}{r^2}\right\rangle = \frac{1}{\left(l+\frac{1}{2}\right)n^3a^2}, \quad \left\langle\frac{1}{r^3}\right\rangle = \frac{1}{l\left(l+\frac{1}{2}\right)(l+1)n^3a^3},} \tag{2.19}$$

and

$$\langle r\rangle = \frac{a}{2}\left[3n^2 - l(l+1)\right], \quad \langle r^2\rangle = \frac{n^2a^2}{2}\left[5n^2 - 3l(l+1) + 1\right]. \tag{2.20}$$

You are bond to use them in perturbation theory of Hydrogen (say, fine structure and Zeeman effect).

2.3 Feynman-Hellmann Theorem

Feynman's bachelor thesis provides one possible proof. Call λ some parameter in Hamiltonian and energy, then

$$\frac{\partial E_n}{\partial\lambda} = \left\langle\psi_n\middle|\frac{\partial H}{\partial\lambda}\middle|\psi_n\right\rangle. \tag{2.21}$$

Alternative proof using perturbation theory: Let the unperturbed Hamiltonian be $H_0 = H(\lambda_0)$ for some fixed value λ_0. Now tweak λ to $\lambda_0 + \mathrm{d}\lambda$, the perturbation Hamiltonian is

$$H' = H(\lambda_0 + \mathrm{d}\lambda) - H(\lambda_0) = \frac{\partial H}{\partial\lambda}\,\mathrm{d}\lambda. \tag{2.22}$$

The variation in energy is given by (evaluated at λ_0)

$$\mathrm{d}E = E_n^{(1)} = \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle = \left\langle\psi_n\middle|\frac{\partial H}{\partial\lambda}\middle|\psi_n\right\rangle, \tag{2.23}$$

hence

$$\frac{\partial E_n}{\partial\lambda} = \left\langle\psi_n\middle|\frac{\partial H}{\partial\lambda}\middle|\psi_n\right\rangle. \tag{2.24}$$

(Q.E.D.)

Time-dependent Feynman-Hellmann theorem:

$$\left\langle\Psi(t)\middle|\frac{\partial H}{\partial\lambda}\middle|\Psi(t)\right\rangle = \mathrm{i}\hbar\frac{\partial}{\partial t}\left\langle\Psi(t)\middle|\frac{\partial\Psi(t)}{\partial\lambda}\right\rangle. \tag{2.25}$$