Table of Useful Integrals, etc.

$$\int_0^\infty e^{-ax^2}\,dx = \frac{1}{2}\left(\frac{\pi}{a}\right)^{1/2}$$

$$\int_0^\infty x e^{-ax^2}\,dx = \frac{1}{2a}$$

$$\int_0^\infty x^2 e^{-ax^2}\,dx = \frac{1}{4a}\left(\frac{\pi}{a}\right)^{1/2}$$

$$\int_0^\infty x^3 e^{-ax^2}\,dx = \frac{1}{2a^2}$$

$$\int_0^\infty x^{2n} e^{-ax^2}\,dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}a^n}\left(\frac{\pi}{a}\right)^{1/2}$$

$$\int_0^\infty x^{2n+1} e^{-ax^2}\,dx = \frac{n!}{2a^{n+1}}$$

$$\int_0^\infty x^n e^{-ax}\,dx = \frac{n!}{a^{n+1}}$$

Integration by Parts:

$$\int_a^b U\,dV = \left[UV\right]_a^b - \int_a^b V\,dU$$

U and *V* are functions of *x*. Integrate from *x* = a to *x* = b

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$$\int \sin(ax)\,dx = -\frac{1}{a}\cos(ax)$$

$$\int \sin^2(ax)\,dx = \frac{x}{2} - \frac{\sin(2ax)}{4a}$$

$$\int \sin^3(ax)\,dx = -\frac{1}{a}\cos(ax) + \frac{1}{3a}\cos^3(ax)$$

$$\int \sin^4(ax)\,dx = \frac{3x}{8} - \frac{3\sin(2ax)}{16a} - \frac{\sin^3(ax)\cos(ax)}{4a}$$

$$\int \sin(ax)\sin(bx)\,dx = \frac{\sin\left[(a-b)x\right]}{2(a-b)} - \frac{\sin\left[(a+b)x\right]}{2(a+b)} \quad \textit{where } a^2 \neq b^2$$

$$\int \cos(ax)\cos(bx)\,dx = \frac{\sin\left[(a-b)x\right]}{2(a-b)} + \frac{\sin\left[(a+b)x\right]}{2(a+b)}$$

$$\int \sin(ax)\cos(bx)\,dx = \frac{-\cos\left[(a-b)x\right]}{2(a-b)} - \frac{\cos\left[(a+b)x\right]}{2(a+b)}$$

$$\int x\sin^2(ax)\,dx = \frac{x^2}{4} - \frac{x\sin(2ax)}{4a} - \frac{\cos(2ax)}{8a^2}$$

$$\int x^2\sin^2(ax)\,dx = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin(2ax) - \frac{x\cos(2ax)}{4a^2}$$

$$\int x\sin(ax)\sin(bx)\,dx = \frac{\cos\left[(a-b)x\right]}{2(a-b)^2} - \frac{\cos\left[(a+b)x\right]}{2(a+b)^2} + \frac{x\sin\left[(a-b)x\right]}{2(a-b)^2} - \frac{x\sin\left[(a+b)x\right]}{2(a+b)^2}$$

$$\int x\sin(ax)\,dx = \frac{\sin(ax)}{a^2} - \frac{x\cos(ax)}{a}$$

$$\int x\cos(ax)\,dx = \frac{x\sin(ax)}{a} + \frac{\cos(ax)}{a^2}$$

$$\int \cos(ax)\,dx = \frac{\sin(ax)}{a}$$

$$\int \cos^2(ax)\,dx = \frac{x}{2} + \frac{\sin(2ax)}{4a}$$

$$\int x^2\cos^2(ax)\,dx = \frac{x^3}{6} + \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin(2ax) + \frac{x\cos(2ax)}{4a^2}$$

$$\int \cos(bx)e^{-ax^2}\,dx = \frac{e^{ax}}{(a^2+b^2)}\left[a\cos(bx) + b\sin(bx)\right]$$

Taylor Series:

$$\sum_{n=0}^{n=\infty} \frac{f^{(n)}(x_o)}{n!}(x - x_o)^n$$

Geometric Series:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$$

Euler's Formula:

$e^{i\phi} = \cos\phi + i\sin\phi$

Quadratic Equation and other higher order polynomials:

$$ax^2 + bx + c = 0$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$ax^4 + bx^2 + c = 0$$

$$x = \pm\left(\frac{-b \pm \sqrt{b^2 - 4ac}}{2a}\right)$$

General Solution for a Second Order Homogeneous Differential Equation with Constant Coefficients:

If: $y'' + py' + qy = 0$

Assume a solution for y:

$$y = e^{sx} \quad y' = se^{sx} \quad y'' = s^2e^{sx}$$

$$\therefore \quad s^2e^{sx} + pse^{sx} + qe^{sx} = 0$$

$$and \quad s^2 + ps + q = 0$$

$$Hence \quad y = c_1e^{s_1x} + c_2e^{s_2x}$$

Conversions from spherical polar coordinates into Cartesian coordinates:

$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$x = r\cos\theta$$

$$dv = r^2\sin\theta dr d\theta d\phi$$

$$0 < r < \infty$$

$$0 < \theta < \pi$$

$$0 < \phi < 2\pi$$

Commutator Identities:

$$\left[\hat{A},\hat{B}\right] = -\left[\hat{B},\hat{A}\right]$$

$$\left[\hat{A},\hat{A}^n\right] = 0 \quad n = 1,2,3,\cdots$$

$$\left[k\hat{A},\hat{B}\right] = \left[\hat{A},k\hat{B}\right] = k\left[\hat{A},\hat{B}\right]$$

$$\left[\hat{A}+\hat{B},\hat{C}\right] = \left[\hat{A},\hat{C}\right] + \left[\hat{B},\hat{C}\right]$$

$$\left[\hat{A},\hat{B}\hat{C}\right] = \left[\hat{A},\hat{B}\right]\hat{C} + \hat{B}\left[\hat{A},\hat{C}\right]$$

$$\left[\hat{A}\hat{B},\hat{C}\right] = \left[\hat{A},\hat{C}\right]\hat{B} + \hat{A}\left[\hat{B},\hat{C}\right]$$

Creation and Annihilation Operators

$$l_\pm\left|l,m_l,s,m_s\right\rangle = \left(l\left(l+1\right) - m_l\left(m_l \pm 1\right)\right)^{1/2}\hbar\left|l,m_{l\pm1},s,m_s\right\rangle$$

$$s_\pm\left|l,m_l,s,m_s\right\rangle = \left(s\left(s+1\right) - m_s\left(m_s \pm 1\right)\right)^{1/2}\hbar\left|l,m_l,s,m_{s\pm1}\right\rangle$$

$$j_\pm\left|j,m_j\right\rangle = \left(j\left(j+1\right) - m_j\left(m_j \pm 1\right)\right)^{1/2}\hbar\left|j,m_{j\pm1}\right\rangle$$

Atomic Units:

Quantity	Atomic unit in cgs or other units	Values of some atomic properties in atomic units (a.u.)
Mass	$m_e = 9.109534 \times 10^{-28}$ g	Mass of electron = 1 a.u.
Length	$a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2$ $= 0.52917706 \times 10^{-10}$ m (= 1 bohr)	Most probable distance of 1s electron from nucleus of H atom = 1 a.u.
Time	$\tau_0 = a_0\hbar/e^2$ $= 2.4189 \times 10^{-17}$ sec	Time for 1s electron in H atom to travel one bohr = 1 a.u.
Charge	$e = 4.803242 \times 10^{-10}$ esu $= 1.6021892 \times 10^{-19}$ coulomb	Charge of electron = −1 a.u.
Energy	$e^2/4\pi\varepsilon_0 a_0 = 4.359814 \times 10^{-18}$ J (= 27.21161 eV ≡ 1 hartree)	Total energy of 1s electron in H atom = −1/2 a.u.
Angular momentum	$\hbar = h/2\pi$ $= 1.0545887 \times 10^{-34}$ J sec	Angular momentum for particle in ring = 0, 1, 2, ... a.u.
Electric field strength	$e/a_0{}^2 = 5.1423 \times 10^9$ V/cm	Electric field strength at distance of 1 bohr from proton = 1 a.u.

Physical Constants:

Values of Some Physical Constants

Constant	Symbol	Value
Atomic mass constant	m_u	$1.660\ 5402 \times 10^{-27}$ kg
Avogadro constant	N_A	$6.022\ 1367 \times 10^{23}$ mol^{-1}
Bohr magneton	$\mu_B = e\hbar/2m_e$	$9.274\ 0154 \times 10^{-24}$ J · T^{-1}
Bohr radius	$a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2$	$5.291\ 772\ 49 \times 10^{-11}$ m
Boltzmann constant	k_B	$1.380\ 658 \times 10^{-23}$ J · K^{-1}
		$0.695\ 038$ cm^{-1}
Electron rest mass	m_e	$9.109\ 3897 \times 10^{-31}$ kg
Gravitational constant	G	$6.672\ 59 \times 10^{-11}$ m^3 · kg^{-1} · s^{-2}
Molar gas constant	R	$8.314\ 510$ J · K^{-1} · mol^{-1}
		$0.083\ 1451$ dm^3 · bar · K^{-1} · mol^{-1}
		$0.082\ 0578$ dm^3 · atm · K^{-1} · mol^{-1}
Molar volume, ideal gas		
(one bar, 0°C)		$22.711\ 08$ L · mol^{-1}
(one atm, 0°C)		$22.414\ 09$ L · mol^{-1}
Nuclear magneton	$\mu_N = e\hbar/2m_p$	$5.050\ 7866 \times 10^{-27}$ J · T^{-1}
Permittivity of vacuum	ε_0	$8.854\ 187\ 816 \times 10^{-12}$ C^2 · J^{-1} · m^{-1}
	$4\pi\varepsilon_0$	$1.112\ 650\ 056 \times 10^{-10}$ C^2 · J^{-1} · m^{-1}
Planck constant	h	$6.626\ 0755 \times 10^{-34}$ J · s
	$\hbar$	$1.054\ 572\ 66 \times 10^{-34}$ J · s
Proton charge	e	$1.602\ 177\ 33 \times 10^{-19}$ C
Proton magnetogyric ratio	γ_p	$2.675\ 221\ 28 \times 10^{8}$ s^{-1} · T^{-1}
Proton rest mass	m_p	$1.672\ 6231 \times 10^{-27}$ kg
Rydberg constant (Bohr)	$R_\infty = m_e e^4/8\varepsilon_0^2 h^2$	$2.179\ 8736 \times 10^{-18}$ J
		$109\ 737.31534$ cm^{-1}
Rydberg constant (exptl)	R_H	$109\ 677.581$ cm^{-1}
Speed of light in vacuum	c	$299\ 792\ 458$ m · s^{-1} (defined)
Stefan–Boltzmann constant	$\sigma = 2\pi^5 k_B^4/15h^3c^2$	$5.670\ 51 \times 10^{-8}$ J · m^{-2} · K^{-4} · s^{-1}

Operators:

TABLE 4.1
Classical-mechanical observables and their corresponding quantum-mechanical operators.

Observable		Operator	
Name	Symbol	Symbol	Operation
Position	x	$\hat{X}$	Multiply by x
	$\mathbf{r}$	$\hat{\mathbf{R}}$	Multiply by $\mathbf{r}$
Momentum	p_x	$\hat{P}_x$	$-i\hbar \frac{\partial}{\partial x}$
	$\mathbf{p}$	$\hat{\mathbf{P}}$	$-i\hbar \left(\mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z} \right)$
Kinetic energy	K_x	$\hat{K}_x$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
	K	$\hat{K}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$
			$= -\frac{\hbar^2}{2m}\nabla^2$
Potential energy	$V(x)$	$\hat{V}(\hat{x})$	Multiply by $V(x)$
	$V(x, y, z)$	$\hat{V}(\hat{x}, \hat{y}, \hat{z})$	Multiply by $V(x, y, z)$
Total energy	E	$\hat{H}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$
			$+ V(x, y, z)$
			$= -\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z)$
Angular momentum	$L_x = yp_z - zp_y$	$\hat{L}_x$	$-i\hbar \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right)$
	$L_y = zp_x - xp_z$	$\hat{L}_y$	$-i\hbar \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right)$
	$L_z = xp_y - yp_x$	$\hat{L}_z$	$-i\hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right)$