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Collection of formulae
Quantum mechanics

Basic Formulas

The de Broglie wave length

$$\lambda = \frac{h}{p}$$

The Schrödinger equation

$$H\psi(\boldsymbol{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t)$$

Stationary states

$$H\psi(\boldsymbol{r},t) = E\psi(\boldsymbol{r},t)$$

$$\psi(\boldsymbol{r},t) = \psi(\boldsymbol{r})\cdot\phi(t), \text{ where } \phi(t) = e^{-iEt/\hbar}$$

The Hamiltonian of one particle

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})$$

Probability flux

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{\hbar}{2im}\left(\psi^*(\boldsymbol{r})\boldsymbol{\nabla}\psi(\boldsymbol{r}) - \psi(\boldsymbol{r})\boldsymbol{\nabla}\psi^*(\boldsymbol{r})\right)$$

Equation of continuity

$$\frac{\partial}{\partial t}P(\boldsymbol{r},t) + \nabla\cdot\boldsymbol{j}(\boldsymbol{r},t) = 0, \text{ where}$$

$$P(\boldsymbol{r},t) = |\psi(\boldsymbol{r},t)|^2 = \psi^*(\boldsymbol{r},t)\psi(\boldsymbol{r},t)$$

Group velocity

$$v_g = \frac{\partial\omega}{\partial k}$$

Operators

Physical quantity	x-representation	p-representation
Position coordinate x	x	$x = i\hbar\frac{\partial}{\partial p_x}$
Position vector $\boldsymbol{r}$	$\boldsymbol{r}$	$i\hbar\nabla_p$
x-component of momentum p_x	$-i\hbar\frac{\partial}{\partial x}$	p_x
Momentum $\boldsymbol{p}$	$-i\hbar\nabla$	$\boldsymbol{p}$
Kinetic Energy $T = \frac{\boldsymbol{p}^2}{2m}$	$-\frac{\hbar^2}{2\mu}\nabla^2$	$\frac{1}{2\mu}P^2$
Potential energy $V(\boldsymbol{r},t)$	$V(\boldsymbol{r},t)$	$V(i\hbar\nabla_p,t)$
Total energy $T = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r},t)$	$-\frac{\hbar^2}{2\mu}\nabla^2 + V(\boldsymbol{r},t)$	$\frac{1}{2\mu}P^2 + V(i\hbar\nabla_p,t)$

Commutator of operator A and B

$$[A,B] = AB - BA$$

Commutator algebra

$$[AB,C] = A[B,C] + [A,C]B$$

$$[A,B+C] = [A,B] + [A,C]$$

$$[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$$

Some usefull commutators

$$[x,p_x] = i\hbar$$

Expectation value

$$\langle A\rangle = \int\psi^* A\psi dV, \text{ where } \psi \text{ is a normalized wave function.}$$

Variance

$$\Delta A = \sqrt{\left\langle(A - \langle A\rangle)^2\right\rangle} = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$$

Uncertainty relation

$$\Delta A\,\Delta B \geq \frac{1}{2}|\,\langle i[A,B]\rangle\,|$$

Time dependence of expectation values

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\langle[H,A]\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle$$

The Expansion theorem

Suppose that $\mathcal{A}$ is a Hermitian operator with discrete eigenfunctions u_n and continuous eigenfunctions u_q. Then the arbitrary function $\psi(x)$ may be expanded in terms of u_n and u_q as

$$\psi(x) = \sum_n c_n u_n$$

where

$$c_n = \int u_n^* \psi = < u_n|\psi >$$

if

$$\int u_n^* u_n = < u_n|u_n >= 1 \text{ and } \int u_m^* u_n = < u_m|u_n >= 0 \text{ if } m \neq n$$

The time dependent solution is given by

$$\Psi(x,t) = \sum_n c_n u_n(x) e^{-iE_n t/\hbar}$$

Hermitian operators

The eigenvalues of a Hermitian operator $\mathcal{A}$ are real, and the eigenfunctions of $\mathcal{A}$ corresponding to different eigenvalues are orthogonal.

Angular Momentum $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$ and Spin

Orbital angular momentum operator

$$\boldsymbol{L} = -i\hbar \boldsymbol{r} \times \nabla$$

$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

Eigenfunctions and eigenvalues to angular momentum operators

The eigenfunction are the spherical harmonics $Y_{lm}(\theta, \phi)$

$$\boldsymbol{L^2} Y_{lm} = \hbar^2 l(l+1) Y_{lm}$$

$$L_z Y_{lm} = m\hbar Y_{lm}$$

Commutator relations of angular momentum operators (and spin)

$$[L_x, L_y] = i\hbar L_z, \text{ with cyclic permutation}$$

$$[\boldsymbol{L}^2, L_z] = [H, L_z] = [H, \boldsymbol{L}^2] = 0$$

Ladder operators for angular momentum (and spin)

$$L_\pm = L_x \pm i L_y$$

$$L_\pm Y_{l,m} = \hbar\sqrt{l(l+1) - m(m\pm 1)}\, Y_{l,m\pm 1}$$

$$[L_z, L_\pm] = \pm\hbar L_\pm$$

$$[L^2, L_\pm] = 0$$

Spin Operators

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

General spin state

$$\chi = a\chi_+ + b\chi_- = \begin{pmatrix} a \\ b \end{pmatrix} \text{ where } \chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Scalar product

$$\langle \chi' | \chi \rangle = (c^* \;\; d^*) \begin{pmatrix} a \\ b \end{pmatrix} = c^* a + d^* b$$

Special Solutions

Tunneling in the WKB approximation

$$|T|^2 \approx \exp\left(-2\int_{\text{barrier}} dx \sqrt{2m[V(x) - E]}/\hbar\right)$$

Tunneling at a potential step and a square barrier

Potential step of height V_0 and particle of mass m incident from the left of energy E, $E > V_0$.

$$k_1 = \frac{1}{\hbar}\sqrt{2mE} \qquad \text{and} \qquad k_2 = \frac{1}{\hbar}\sqrt{2m(E - V_0)}$$

The transmission coefficient T is

$$T = \frac{\mid S_{\text{transmitted}} \mid}{\mid S_{\text{incident}} \mid} = \frac{4k_1 k_2}{(k_1 + k_2)^2} \text{ and}$$

$$R = \frac{\mid S_{\text{reflected}} \mid}{\mid S_{\text{incident}} \mid} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

where S is probability flux.

$$T + R = 1$$

Potential barrier of height V_0 and width a and particle of mass m incident from the left of energy E, $E > V_0$.

$$T = \left[1 + \frac{V_0^2 \sinh^2(\alpha a)}{4E(V_0 - E)}\right]^{-1} \qquad \text{if} \qquad (E < V_0)$$

$$T = \left[1 + \frac{V_0^2 \sin^2(\alpha a)}{4E(E - V_0)}\right]^{-1} \qquad \text{if} \qquad (E > V_0)$$

$$\alpha = \frac{\sqrt{2m \mid V_0 - E \mid}}{\hbar}$$

Particle in a square potential
The potential is $V(x) = 0$ for $0 < x < a$ and infinite elsewhere.

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$\psi(x) = \sqrt{\frac{2}{a}}\ \sin(\frac{n\pi x}{a})$$

Density of one-particle states in a box of volume V
As a function of energy

$$g(\boldsymbol{E}) d^3p = \frac{V}{(6\pi^2)} \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{3}{2}\sqrt{E} \qquad \text{Note: No spin}$$

The Fermi energy

$$E_F = \left(\frac{N}{V} 3\pi^2\right)^{2/3} \frac{\hbar^2}{2m}$$

The Fermi velocity

$$v_F = \sqrt{\frac{2E_F}{m}}$$

Linear harmonic oscillator (in 1d)

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$$

$$H = \frac{\hbar^2}{2m}\nabla^2 + V(x) \;=\; \frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}kx^2 \;=\; \frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 x^2$$

Ladder operators for the harmonic oscillator

$$a_+ = \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x) \text{ and } a_- = \frac{1}{\sqrt{2\hbar m\omega}}(+ip + m\omega x)$$

The inverse is

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-) \text{ and } p = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ + a_-)$$

The action of a ladder operator on an eigenfunction

$$a_+\psi_n = \sqrt{n+1}\ \psi_{n+1} \quad \text{and} \quad a_-\psi_n = \sqrt{n}\ \psi_{n-1}$$

The commutstor of a_+ and a_- is

$$[a_-, a_+] = 1$$

$$H = \hbar\omega\left(a_+a_- + \frac{1}{2}\right) = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$u_n(x) = C_n H_n(\frac{x}{b}) \exp\left(-\frac{x^2}{2b^2}\right),$$

where $H_n(x) =$ Hermite polynomial of order n, and

$$C_n = \left(\frac{1}{2^n n!}\right)^{1/2} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}, b = \sqrt{\frac{\hbar}{m\omega}}.$$

The eigenfunctions $u_n(x)$ of the harmonic oscillator satisfy the following recursion relation

$$x u_n(x) = \frac{b}{\sqrt{2}}\left(\sqrt{n+1}\, u_{n+1}(x) + \sqrt{n}\, u_{n-1}(x)\right),$$

$$x^2 u_n(x) = \frac{b^2}{2}\left(\sqrt{(n+1)(n+2)}\, u_{n+2}(x) + (2n+1)u_n(x) + \sqrt{n(n-1)}\, u_{n-2}(x)\right).$$

The Hermite polynomials satisfy the following recursion relation

$$H_{n+1}(\xi) - 2\xi H_n(\xi) + 2nH_{n-1}(\xi) = 0$$

Hermite polynomials

n	$H_n(x)$
0	$H_0(x) = 1$
1	$H_1(x) = 2x$
2	$H_2(x) = 4x^2 - 2$
3	$H_3(x) = 8x^3 - 12x$
4	$H_4(x) = 16x^4 - 48x^2 + 12$

Eigenfunctions of the harmonic oscillator

n	$\psi_n(x)$ where $\alpha = \sqrt{m\omega/\hbar}$
0	$\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}\alpha^2x^2}$
1	$\psi_1(x) = \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} 2\alpha x e^{-\frac{1}{2}\alpha^2x^2}$
2	$\psi_2(x) = \left(\frac{\alpha}{8\sqrt{\pi}}\right)^{1/2} (4\alpha^2x^2 - 2)e^{-\frac{1}{2}\alpha^2x^2}$
3	$\psi_3(x) = \left(\frac{\alpha}{48\sqrt{\pi}}\right)^{1/2} (8\alpha^3x^3 - 12\alpha x)e^{-\frac{1}{2}\alpha^2x^2}$
4	$\psi_4(x) = \left(\frac{\alpha}{384\sqrt{\pi}}\right)^{1/2} (16\alpha^4x^4 - 48\alpha^2x^2 + 12)e^{-\frac{1}{2}\alpha^2x^2}$
5	$\psi_5(x) = \left(\frac{\alpha}{3840\sqrt{\pi}}\right)^{1/2} (32\alpha^5x^5 - 160\alpha^3x^3 + 120\alpha x)e^{-\frac{1}{2}\alpha^2x^2}$

Hydrogenic Atoms

The Schrödinger equation in spherical coordinates

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r\cdot + \frac{\boldsymbol{L}^2}{2mr^2} + V(r)\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

Spherical harmonics $Y_{l,m}(\theta,\phi)$ (Klotytefunktioner)

l	m	$Y_{l,m}(\theta,\phi)$
0	0	$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$
1	0	$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta$
1	±1	$Y_{1,\pm1} = \mp\sqrt{\frac{3}{8\pi}}e^{\pm i\phi}\sin\theta$
2	0	$Y_{2,0} = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$
2	±1	$Y_{2,\pm1} = \mp\sqrt{\frac{15}{8\pi}}e^{\pm i\phi}\sin\theta\cos\theta$
2	±2	$Y_{2,\pm2} = \sqrt{\frac{15}{32\pi}}e^{\pm 2i\phi}\sin^2\theta$
3	0	$Y_{3,0} = \sqrt{\frac{7}{16\pi}}\left(5\cos^3\theta - 3\cos\theta\right)$
3	±1	$Y_{3,\pm1} = \mp\sqrt{\frac{21}{64\pi}}\sin\theta\left(5\cos^2\theta - 1\right)e^{\pm i\phi}$
3	±2	$Y_{3,\pm2} = \sqrt{\frac{105}{32\pi}}\sin^2\theta\cos\theta\, e^{\pm 2i\phi}$
3	±3	$Y_{3,\pm3} = \mp\sqrt{\frac{35}{64\pi}}\sin^3\theta\, e^{\pm 3i\phi}$

$$Y_{l,-m} = (-1)^m Y^*_{l,m}$$

Radial wave functions of hydrogenic atoms

n	l	$R_{n,l}(r)$
1	0	$R_{1,0}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	$R_{2,0}(r) = 2\left(\frac{Z}{2a_0}\right)^{3/2}\left(1 - \frac{Zr}{2a_0}\right)e^{-Zr/2a_0}$
2	1	$R_{2,1}(r) = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}$
3	0	$R_{3,0}(r) = 2\left(\frac{Z}{3a_0}\right)^{3/2}\left(1 - \frac{2Zr}{3a_0} + \frac{2(Zr)^2}{27a_0^2}\right)e^{-Zr/3a_0}$
3	1	$R_{3,1}(r) = \frac{4\sqrt{2}}{3}\left(\frac{Z}{3a_0}\right)^{3/2}\frac{Zr}{a_0}\left(1 - \frac{Zr}{6a_0}\right)e^{-Zr/3a_0}$
3	2	$R_{3,2}(r) = \frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Z}{3a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$
4	0	$R_{4,0}(r) = 2\left(\frac{Z}{4a_0}\right)^{3/2}\left(1 - \frac{3Zr}{4a_0} + \frac{(Zr)^2}{8a_0^2} - \frac{(Zr)^3}{192a_0^3}\right)e^{-Zr/4a_0}$

Associated Laguerre polynomials

$L_n^\alpha(x)$		
$L_1^1(x)$	$=$	-1
$L_2^1(x)$	$=$	$2x-4$
$L_2^2(x)$	$=$	2
$L_3^1(x)$	$=$	$-3x^2+18x-18$
$L_3^2(x)$	$=$	$-6x+18$
$L_3^3(x)$	$=$	-6

Expectation values of r^k in hydrogenic atoms

$$\langle r\rangle = \frac{1}{2}\left[3n^2-l(l+1)\right]\left(\frac{a_0}{Z}\right)$$

$$\langle r^2\rangle = \frac{n^2}{2}\left[5n^2+1-3l(l+1)\right]\left(\frac{a_0}{Z}\right)^2$$

$$\langle r^{-1}\rangle = \frac{1}{n^2}\left(\frac{Z}{a_0}\right)$$

$$\langle r^{-2}\rangle = \frac{2}{n^3(2l+1)}\left(\frac{Z}{a_0}\right)^2$$

$$\langle r^{-3}\rangle = \frac{1}{n^3 l(l+\frac{1}{2})(l+1)}\left(\frac{Z}{a_0}\right)^3$$

Energy of a diatomic molecule

$$E = E_{trans}+E_{vib}+E_{rot} = \frac{p^2}{2m}+\hbar\omega(n+\frac{1}{2})+\frac{\hbar^2}{2I}l(l+1) \qquad (1)$$

where I is the moment of inertia. In case of a diatomic molecule this equates to $I=\mu R^2=\frac{m_C m_O}{m_C+m_O}R^2$.

Electrical dipol radiation

Transition rules

$$\Delta l = \pm 1 \text{ and } \Delta m_l = \pm 1 \text{ or } 0$$

For a harmonic oscillator model of a diatomic molecule (see equation 1):

$$\Delta l = \pm 1 \text{ and } \Delta n = \pm 1 \text{ or } 0$$

Perturbation Theory

The Hamiltonian $H=H_0+H_1$ where H_0 is the un perturbed Hamiltonian with a known solution ϕ_n and H_1 is the perturbation.
First order perturbation

$$E_n^{(1)} =< \phi_n|H_1|\phi_n >$$

$$\psi_n^{(1)} = \phi_n + \sum_{k\neq n}\frac{< \phi_k|H_1|\phi_n >}{E_n^0-E_k^0}\,\phi_k$$

Second order perturbation

$$E_n^{(2)} = \sum_{k\neq n}\frac{|< \phi_k|H_1|\phi_n >|^2}{E_n^0-E_k^0}$$

First order perturbation, time dependent The transition rate from state a to state b is given by:

$$P_{ba}(t) = | c_b(t) |^2$$

where

$$c_b(t) = \frac{1}{i\hbar}\int_{t_0}^{t}\langle\psi_b \mid H_1(t) \mid \psi_a\rangle e^{i\omega_{ba}t}dt$$

where

$$\omega_{ba}t = \frac{E_b-E_a}{\hbar}$$

Statistical Physics

The Boltzmann factor for a stat of energy E_i

$$P_i \propto \exp(-E_i/k_BT)$$

The Partition function (Tillståndssumman)

$$Z = \sum_j \exp(-E_j/k_BT)$$

and hence

$$P_i = \frac{\exp(-E_i/k_BT)}{Z}$$

Expectation value of n for a harmonic oscillator

$$\langle n \rangle = \frac{1}{\exp(\hbar\omega/k_B T) - 1}$$

The average energy of a quadratic degree of freedom

$$< E >= \frac{1}{2} k_B T$$

Many Identical particles

The Fermi energy is given by:

$$E_F = \left(\frac{N}{V} 3\pi^2 \right)^{2/3} \frac{\hbar^2}{2m}$$

Total energy of e Fermi gas:

$$E_{tot} = \frac{3}{5} N E_F$$

The density of states (spinless) is given by:

$$D(\epsilon) = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{2/3} \sqrt{\epsilon}$$

Slater determinant:

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_\alpha(r_1) & \psi_\beta(r_1) & .. & \psi_\omega(r_1) \\ \psi_\alpha(r_2) & \psi_\beta(r_2) & .. & \psi_\omega(r_2) \\ .. & .. & .. & .. \\ \psi_\alpha(r_n) & \psi_\beta(r_n) & .. & \psi_\omega(r_n) \end{vmatrix}$$