Noter til KM1 på KU (Kvantemekanik 1)

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Indhold

Introduktion

Fundamentale ligninger

Schrödingerligningen	$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$
Tidsuafhængige Schrödingerligning	$H\psi = E\psi, \quad \Psi = \psi e^{-iEt/\hbar}$
Hamiltonoperator	$H = -\frac{\hbar^2}{2m}\nabla^2 + V$
Impulsoperator	$\mathbf{p} = -i\hbar\nabla$
Tidsafhængighed af forventningsværdi	$\frac{d\langle Q\rangle}{dt} = \frac{i}{\hbar}\langle[H,Q]\rangle + \left\langle\frac{\partial Q}{\partial t}\right\rangle$
Generaliseret usikkerhedsrelation	$\sigma_A\sigma_B \geq \left\lvert\frac{1}{2i}\langle[A,B]\rangle\right\rvert$
Heisenbergs usikkerhedsrelation	$\sigma_x\sigma_p \geq \hbar/2$
Kanonisk kommutator	$[x,p] = i\hbar$
Angulært moment	$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y$
Paulimatricer	$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

Fundamentale konstante

Planks (reducerede) konstant	$\hbar$	=	$1.05457 \cdot 10^{-34}$ J s
Lysets hastighed	c	=	$2.99792 \cdot 10^{8}$ m/s
Elektronmasse	m_e	=	$9.10938 \cdot 10^{-31}$ kg
Protonmasse	m_p	=	$1.67262 \cdot 10^{-27}$ kg
Elementarladning	e	=	$1.60218 \cdot 10^{-19}$ C
Vakuumpermitivitet	ϵ_0	=	$8.85419 \cdot 10^{-12}$ C^2/ J m
Boltzmannkonstanten	k_B	=	$1.38065 \cdot 10^{-23}$ J/K

Hydrogenatomet

Finstrukturkonstanten	α	$=$	$\dfrac{e^2}{4\pi\epsilon_0\hbar c}$	$=$	$1/137.036$
Bohrradius	a	$=$	$\dfrac{4\pi\epsilon_0\hbar^2}{m_e e^2} = \dfrac{\hbar}{\alpha m_e c}$	$=$	$5.29177 \cdot 10^{-11}$ m
Bohrenergier	E_n	$=$	$-\dfrac{m_e e^4}{2(4\pi\epsilon_0)^2\hbar^2 n^2}$	$=$	$\dfrac{E_1}{n^2}$ $(n = 1, 2, 3, ...)$
Bindingsenergi	$-E_1$	$=$	$\dfrac{\hbar^2}{2m_e a^2} = \dfrac{\alpha^2 m_e c^2}{2}$	$=$	13.6057 eV
Grundstadie	ψ_0	$=$	$\dfrac{1}{\sqrt{\pi a^3}} e^{-r/a}$		
Rydbergformlen	$\dfrac{1}{\lambda}$	$=$	$R\left(\dfrac{1}{n_f^2} - \dfrac{1}{n_i^2}\right)$		
Rydbergkonstanten	R	$=$	$-\dfrac{E_1}{2\pi\hbar c}$	$=$	$1.09737 \cdot 10^7$ m^{-1}

Matematiske formler

Trigonometri

$$\sin(a \pm b) = \sin a \cos b \pm \cos a \sin b$$
$$\cos(a \pm b) = \cos a \cos b \mp \sin a \sin b$$

Cosinusrelationen (c er siden over for vinklen θ)

$$c^2 = a^2 + b^2 - 2ab\cos\theta$$

Integraler

$$\int x \sin ax \ \mathrm{d}x = \frac{1}{a^2}\sin ax - \frac{x}{a}\cos ax$$
$$\int x \cos ax \ \mathrm{d}x = \frac{1}{a^2}\cos ax + \frac{x}{a}\sin ax$$

Eksponentielle integraler

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

Gaussiske integraler

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

Partiel integration (produktreglen for differentiation, baglens)

$$\int_a^b f\frac{dg}{dx} \ \mathrm{d}x = -\int_a^b \frac{df}{dx} g \ \mathrm{d}x + [fg]_a^b$$

1 Bølgefunktionen

1.1 Schrödingerligningen