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Välikokeen kaavakokoelma

ı-kentän yhtälöitä

$$= q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}),$$

$$= \frac{1}{2}\varepsilon_0 E^2 + \frac{1}{2\mu_0} B^2,$$

$$= 1/\sqrt{\varepsilon_0 \mu_0}.$$

ıtonien ominaisuuksia

$$= hf$$

$$= cp$$

$$= \hbar k$$

$$= \lambda f$$

$$\frac{J}{f} = \frac{8\pi h f^3}{c^3} \frac{V}{e^{hf/k_B T} - 1},$$

$$_{ot} = \int_0^\infty U(f)\,df = \frac{8\pi h V}{c^3} \int_0^\infty \frac{f^3}{e^{hf/kT} - 1}\,df.$$

$$_{ot} = aT^4, \quad a = 8\pi^5 k^4 / \left(15 c^3 h^3\right)$$

ılosähköinen ilmiö

$$_{,} = E - \phi.$$

$$_{,} = hf - \phi$$

$$E_{kin} = h\frac{c}{\lambda} - \phi$$

$$_{,max} = hf - \phi.$$

$$'_0 = hf - \phi_0.$$

ımptonin ilmiö

$$= c\sqrt{m_e^2 c^2 + p^2}.$$

$$= \boldsymbol{p}' + \boldsymbol{p}_e$$

$$+ m_e c^2 = E' + c\sqrt{m_e^2 c^2 + p_e^2}.$$

$$- \lambda = \lambda_c (1 - \cos\theta)$$

ıffraktio

$$l \sin\theta = n\lambda$$

ıltoliike

$$_{hase} = \lambda f = \frac{\omega}{k}.$$

$$v_{group} = \frac{\quad}{dk}.$$

Aineaallot

$$\lambda = h/p$$

$$p = \frac{h}{2\pi} k = \hbar k$$

$$E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}.$$

$$v_{group} = \frac{d\omega}{dk} = p/m = v$$

$$v_{phase} = \frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{1}{2} v$$

Epämääräisyysperiaate

$$\Delta p \Delta x \geq \hbar/2 \quad \Delta t \Delta E \geq \hbar/2$$

$$\Delta Q = \sqrt{\frac{\sum_i (Q_i - \bar{Q})^2 n_i}{\sum_i n_i}}$$

$$\Delta Q = \sqrt{\left[\overline{Q^2} - (\bar{Q})^2\right]}$$

Todennäköisyystiheys

$$P(x) = |\psi(x)|^2.$$

$$P(\boldsymbol{r}) = |\psi(x,y,z)|^2.$$

$$\int_{\substack{\text{koko}\\ \text{avaruus}}} |\psi(x,y,z)|^2\, dx\,dy\,dz = 1.$$

Schrödingerin yhtälö

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + U(x,y,z)\psi = E\psi.$$

Ajasta riippuva yhtälö

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + U(x,y,z)\psi = i\hbar\frac{\partial\psi}{\partial t}.$$

Vapaalle hiukkaselle

$$\frac{\psi}{x^2}+k^2\psi=0 \quad , k=\sqrt{\frac{\ldots}{\hbar^2}},\ U=0.$$

$$\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)=E\psi .$$

$$(x)=Ae^{ikx}+Be^{-ikx}.$$

hrin malli

$$r=n\lambda, \qquad rp=m_e rv=nh/2\pi \qquad L=n\hbar .$$

$$\frac{{}_e v^2}{r}=\frac{Ze^2}{4\pi\varepsilon_0 r^2}.$$

$$=\frac{n^2h^2\varepsilon_0}{\pi m_e Ze^2}=\frac{n^2}{Z}a_0 \quad \text{missä } a_0=\frac{h^2\varepsilon_0}{\pi m_e e^2}=5,2917\times10^{-11}\,\text{m},$$

$$=-\frac{m_e e^4Z^2}{8\varepsilon_0^2h^2n^2} \quad ; \quad n=1,2,3,..$$

$$-E_1=\left(-\frac{RhcZ^2}{n_2^2}\right)-\left(\frac{RhcZ^2}{n_1^2}\right)=RhcZ^2\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right).$$

$$=\frac{E_2-E_1}{h}=RcZ^2\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right)=3,2899\times10^{15}Z^2\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right)\text{Hz}.$$

ltopaketti

$$(x)=\int_{-\infty}^{\infty}A(k)e^{ikx}dk,$$

$$(k)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\psi(x)e^{-ikx}dx$$

ationäärinen tila

$$(x,t)=\psi(x)e^{-iEt/\hbar},$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi$$

$$(x,t)\Big|^2=\left[\psi^*(x)e^{iEt/\hbar}\right]\left[\psi(x)e^{-iEt/\hbar}\right]=|\psi(x)|^2$$

Potentiaalilaatikko

$$=\left(p_x^2+p_y^2+p_z^2\right)\Big/2m=\frac{\pi^2\hbar^2}{2m}\left(\frac{n_1^2}{a^2}+\frac{n_2^2}{b^2}+\frac{n_3^2}{c^2}\right).$$

$$=C\sin\frac{n_1\pi x}{a}\sin\frac{n_2\pi y}{b}\sin\frac{n_3\pi z}{c}.$$

$$E)=\frac{m^{3/2}V}{2^{1/2}\pi^2\hbar^3}E^{1/2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\tfrac{1}{2}kx^2\psi=E\psi .$$

$$E_n=\left(n+\tfrac{1}{2}\right)\hbar\omega_0,$$

$$E_n=\left(n+\tfrac{3}{2}\right)\hbar\omega_0.$$

$$\omega_0=\sqrt{\frac{k}{m}}$$

Ominaistilat:

n	E_n	$\psi_n(x)$
0	$\frac{1}{2}\hbar\omega_0$	$\psi(x)=(\alpha/\sqrt{\pi})^{1/2}e^{-\alpha^2x^2/2}$
1	$\frac{3}{2}\hbar\omega_0$	$\psi(x)=(\alpha/2\sqrt{\pi})^{1/2}2\alpha xe^{-\alpha^2x^2/2}$
2	$\frac{5}{2}\hbar\omega_0$	$\psi(x)=(\alpha/8\sqrt{\pi})^{1/2}(4\alpha^2x^2-2)e^{-\alpha^2x}$
3	$\frac{7}{2}\hbar\omega_0$	$\psi(x)=(\alpha/48\sqrt{\pi})^{1/2}(8\alpha^3x^3-12\alpha x)e^{-}$

$$\alpha^2=\sqrt{mk}/\hbar=m\omega_0/\hbar$$

Äärellinen potentiaalikuoppa parilliset tilat

$$\tan\sqrt{\frac{ma^2}{2\hbar^2}E}=\sqrt{\frac{U_0-E}{E}}.$$

Äärellinen potentiaalikuoppa parittomat tilat

$$\cot\sqrt{\frac{ma^2}{2\hbar^2}E}=-\sqrt{\frac{U_0-E}{E}}.$$

Operaattorit, odotusarvot ominaisarvot

$$\left[\frac{1}{2m}\left(-\hbar^2\frac{d^2}{dx^2}\right)+U(x)\right]\psi(x)=E\psi(x).$$

$$\hat{H}=\frac{1}{2m}\left(-\hbar^2\frac{d^2}{dx^2}\right)+U(x),$$

Hermiittisyys: $\int_{-\infty}^{\infty}\Phi_1^*\hat{A}\Phi_2dx=\int_{-\infty}^{\infty}\left(\hat{A}\Phi_1\right)^*\Phi_2dx$

$$\hat{H}\psi(x)=E\psi(x).$$

$$\hat{A}\phi_i(x)=a_i\phi_i(x) \qquad i=1,2,\ldots$$

$$\int_{\text{koko avaruus}}\phi_i^*\phi_jdx=\delta_{ij},$$

$$\boldsymbol{p}\to-i\hbar\nabla \qquad \hat{\boldsymbol{L}}=\boldsymbol{r}\times(-i\hbar\nabla)$$

ominaisfunktio e^{ikx} ; ominaisarvo $\hbar k$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+U(r)\psi\ .$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+U(r)\psi=E\psi\ ,$$

$$A_{ave}=\overline{A}=\frac{\int\Phi^*\hat{A}\Phi d^3r}{\int\Phi^*\Phi d^3r}$$

imerkki $\overline{x}=\int\limits_{allspace} x\left|\psi(x)\right|^2 dx$; (jos $\int\limits_{allspace}\left|\psi(x)\right|^2 dx=1$)

ronta ja läpäisy potentiaalivallille (välillä [0,L])

$>U_0$

ue I (x<0),

$$\left(\frac{d^2}{dx^2}+k^2\right)\psi=0 \quad \text{ratkaisu } \psi_I=Ae^{ikx}+Be^{-ikx}.$$

ue II (0<x<L),

$$\left(\frac{d^2}{dx^2}+k'^2\right)\psi=0,\ \text{ratkaisu } \psi_{II}=Ce^{ik'x}+De^{-ik'x}.$$

ue III (L<x)

$$\psi_{III}=Ee^{ikx}.$$

$$=0\quad\begin{cases}A+B=C+D\\ ik(A-B)=ik'(C-D)\end{cases}$$

$$=a\quad\begin{cases}Ce^{ik'a}+De^{-ik'a}=Ee^{ika}\\ ik'(Ce^{ik'a}-De^{-ik'a})=ikEe^{ika}.\end{cases}$$

$$=\frac{k}{k}\frac{|E|^2}{|A|^2}\frac{1}{1+\frac{1}{4}\frac{U_0^2}{E(E-U_0)}\sin^2\sqrt{\frac{2m(E-U_0)}{\hbar^2}}L}.$$

ronta ja läpäisy potentiaalivallille (välillä [0,L])

$<U_0$

$$T=\frac{1}{1+\frac{1}{4}\frac{E_0^2}{E(E_0-E)}\sinh^2\sqrt{\frac{2m(E_0-E)}{\hbar^2}}a}.$$

Kulmaliikemäärä

$$L^2=l(l+1)\hbar^2,\qquad l=0,1,2,3,...$$

$$L_z=m_l\hbar, m_l=-l,-l+1,..,+l\ ,$$

$$\Delta L_x\Delta L_y\geq\tfrac{1}{2}\hbar L_z\ .$$

$$L_\perp^2=(l-1)l\hbar^2=\left(l^2-l\right)\hbar^2.$$

$$\hat{L}=-i\hbar\boldsymbol{r}\times\nabla=-i\hbar\begin{vmatrix}\boldsymbol{u}_x & \boldsymbol{u}_y & \boldsymbol{u}_z\\ x & y & z\\ \partial/\partial x & \partial/\partial y & \partial/\partial z\end{vmatrix}.$$

$$\hat{L}_z=-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right).$$

$$\frac{\partial}{\partial\phi}=\frac{\partial x}{\partial\phi}\frac{\partial}{\partial x}+\frac{\partial y}{\partial\phi}\frac{\partial}{\partial y}+\frac{\partial z}{\partial\phi}\frac{\partial}{\partial z}.$$

$$\hat{L}_z=-i\hbar\frac{\partial}{\partial\phi}.$$

$$-i\hbar\frac{\partial\Phi}{\partial\phi}=A\Phi\ \text{ tai }\ \frac{\partial\Phi}{\partial\phi}=im_l\Phi\ ,$$

$$\int_0^{2\pi}\left(C^*e^{-im_l\phi}\right)\left(Ce^{im_l\phi}\right)d\phi=|C|^2\int_0^{2\pi}d\phi=2\pi|C|^2=1,$$

$$\Phi(\phi)=\frac{1}{\sqrt{2\pi}}e^{im_l\phi},\ m_l=0,\pm1,\pm2,....$$

$$\hat{L}^2=-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right].$$

$$\hat{L}^2Y_{lm_l}=l(l+1)\hbar^2Y_{lm_l}\quad\text{ ja }\quad\hat{L}_zY_{lm_l}=m_l\hbar Y_{lm_l}$$

$$\int\limits_{\substack{\text{Koko}\\ \text{avaruus-}\\ \text{kulma}}}Y_{lm_l}^*Y_{l'm_l'}d\Omega=\int_0^{2\pi}\left(\int_0^{\pi}Y_{lm_l}^*Y_{l'm_l'}\sin\theta d\theta\right)d\phi=\delta_{ll'}\delta_{m_lm_l'}$$

Radiaalinen tod tiheys $P(r)=r^2R_{nl}^2(r)$

Sähködipolitransitiot

...: $\Delta l = \pm 1$, $\Delta m_l = 0, \pm 1$, pariteetin $(-1)^l$ tulee
uuttua.

...nissiotodennäköisyys/aikayksikköä kohden $\approx \dfrac{p^2\omega^3}{12\varepsilon_0 c^3 \hbar}$

$$= e\left| \int_{allspace} r\psi_f^*(r)\psi(r)_i \, dV \right|$$

...taliikkeen magneettinen momentti

$$= -\frac{e}{2m_e}\boldsymbol{L} \quad \mu_{L_z} = -\frac{e}{2m_e}L_z .$$

$$= -\frac{e\hbar}{2m_e}m_l = -\mu_B m_l, \qquad m_l = -l, -l+1, \ldots, +l$$

$$= \frac{e\hbar}{2m_e} \approx 9{,}2740\times10^{-24}\,\mathrm{JT^{-1}} \approx 5{,}7884\times10^{-5}\,\mathrm{eVT^{-1}}$$

$$= |\boldsymbol{\tau}\times\boldsymbol{B}| \rightarrow \left|\frac{d\boldsymbol{L}}{dt}\right| = \left|-\frac{e}{2m_e}\boldsymbol{L}\times\boldsymbol{B}\right|$$

...in ominaisfunktiot ja spinmagneettinen momentti

$$= s(s+1)\hbar^2 = \tfrac{3}{4}\hbar^2 .$$

$$\chi_{m_s} = \tfrac{3}{4}\hbar^2\chi_{m_s} \quad \hat{\boldsymbol{S}}_z\chi_{m_s} = m_s\hbar\chi_{m_s}$$

$$= -g_S\frac{e}{2m_e}\boldsymbol{S} \approx -\frac{e}{m_e}\boldsymbol{S},$$

$|\mu_S| = g_S\mu_B\sqrt{\ldots} \rightarrow \mu_{Sz} = g_S\mu_B m_s$

Sternin ja Gerlachin koe

$$U = -\boldsymbol{\mu}\cdot\boldsymbol{B}$$

$$\boldsymbol{F} = -\nabla(-\boldsymbol{\mu}\cdot\boldsymbol{B}) \quad \boldsymbol{F} = \mu_z\frac{\partial B_z}{\partial z}\hat{z}$$

$$\boldsymbol{F} = \left(-\frac{e}{2m_e}L_z\right)\frac{\partial B_z}{\partial z}\hat{z}$$

$$\boldsymbol{F} = \left(-\frac{em_l\hbar}{2m_e}\right)\frac{\partial B_z}{\partial z}\hat{z}; \quad m_l = -l, -l+1, \ldots, +l$$

$$\boldsymbol{F} = \left(-\frac{e}{m_e}S_z\right)\frac{\partial B_z}{\partial z}\hat{z}$$

$$\boldsymbol{F} = \left(-\frac{em_s\hbar}{m_e}\right)\frac{\partial B_z}{\partial z}\hat{z}; \quad m_s = -s, -s+1, \ldots, +s$$

Spin-orbitaali

$$\psi_{nlm_lm_s} = R_{nl}(r)Y_{lm_l}(\theta,\phi)\chi_{m_s}$$

$$\psi_{nlm_l+\frac{1}{2}} = R_{nl}(r)Y_{lm_l}(\theta,\phi)\uparrow \quad \text{spin up}$$

$$\psi_{nlm_l-\frac{1}{2}} = R_{nl}(r)Y_{lm_l}(\theta,\phi)\downarrow \quad \text{spin down}$$

...tyatomi

$$(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r},$$

$$\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) - \frac{Ze^2}{4\pi\varepsilon_0 r}\psi = E\psi$$

$$(r,\theta,\phi) = R(r)Y(\theta,\phi) \quad \psi_{nlm_l}(r,\theta,\phi) = R_{nl}(r)Y_{lm_l}(\theta,\phi)$$

$$_{eff} = U(r) + \frac{L^2}{2mr^2} = U + \frac{l(l+1)\hbar^2}{2mr^2}$$

$$\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + U(r)\psi = E\psi$$

$$\frac{\hbar^2}{2m_e}\nabla^2\psi + U(r)\psi = E\psi$$

$$\ldots \frac{\partial}{r\,\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\Bigg\}\psi + E_p(r)\psi = E\psi$$

$$\ldots\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\hat{L}^2}{\hbar^2 r^2}\Bigg)\psi + U(r)\psi = E\psi\ .$$

$$\ldots\frac{\ldots}{2m_e}\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right]R_{nl}(r) + U(r)\,R_{nl}(r) = E_n R(r)\,.$$