Ko iščeš ta list, bo s 50% verjetnostjo izginil iz obstoja ali pa razpadel na dva visokoenergijska nevtrina.

Harmonski oscilator:
Harmosnki oscilator opiše hamiltonian $\hat{H} = \frac{\hat{p}}{2m} + \frac{1}{2}k\hat{x}^2 = \frac{\hat{p}}{2m} + \frac{m\omega^2}{2}\hat{x}^2$.
Lastna stanja imajo energijo $E_n = \hbar\omega(n+1/2), \omega^2 = k/m$
Lastne funkcije (so ONS): $\psi_n = \frac{1}{\sqrt{2^n n!\sqrt{\pi}x_0}} e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2} H_n\left(\frac{x}{x_0}\right)$, H_n so Hermitovi polinomi, $x_0 = \sqrt{\frac{\hbar}{m\omega}}$.
Velja še: $x\psi_n = \sqrt{\frac{n+1}{2}}x_0\psi_{n+1} + \sqrt{\frac{n}{2}}x_0\psi_{n-1}$ Verjetnostni tok: $j = \frac{\hbar}{2mi}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)$
Če $\psi = \sum_n a_n\psi_n$, je $a_n = \langle\psi_n, \psi\rangle$, veljati mora $\sum_n |a_n|^2 = 1$, povprečna energija je $E = \sum_n |a_n|^2 E_n$ (in je neodvisna od časa). Verjetnost, da pri meritvi izmerimo energijo E_k je enaka $|a_k|^2$.
$\langle k|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{k,n-1} + \sqrt{n+1}\delta_{k,n+1})$, $\left\langle n|\hat{x^2}|n\right\rangle = \frac{\hbar}{m\omega}(n+\frac{1}{2})$

Hermitovi polinomi: H_{2n} so sodi, H_{2n+1} so lihi.
Velja: $H_n''(u) - 2uH_n'(u) + 2nH_n(u) = 0, H_n'(u) = 2nH_{n-1}(u)$, $\int_{-\infty}^{\infty} e^{-u^2}H_n(u)H_m(u)du = \sqrt{\pi}2^n n!\delta_{n,m}$.
Rekurzivna zveza: $H_{n+1}(u) = 2uH_n(u) - H_n'(u)$, eksplicitni izraz: $H_n(u) = (-1)^n e^{u^2}\frac{d^n}{du^n}e^{-u^2} = \left(2u - \frac{d}{du}\right)^n 1$
$H_0 = 1, H_1 = 2u, H_2 = 4u^2 - 2, H_3 = 8u^3 - 12u, H_4 = 16u^4 - 48u^2 + 12, H_5 = 32u^5 - 160u^3 + 120u$.
$\int_{-\infty}^{\infty} H_n(y)\exp(-y^2 + yy_0 - \frac{y_0^2}{2})dy = \sqrt{\pi}y_0^n\exp(\frac{-y_0^2}{4})$

3D (vrtilna količina):
$\hat{\boldsymbol{p}}\psi = -i\hbar\nabla\psi$, $\hat{\boldsymbol{r}}\psi = (x\psi, y\psi, z\psi)$, $\hat{T} = -\frac{\hbar}{2m}\nabla^2$, $\hat{H} = \hat{T} + \hat{V}$. Predpostavimo $V = V(r)$. $\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}} = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}, z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}, x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$.
Velja: $[L_x, L_y] = i\hbar L_z$ in ciklično. $[L^2, L_i] = 0$.
V sferičnih koordinatah: $x = r\cos\varphi\sin\vartheta, y = \sin\varphi\sin\vartheta, z = r\cos\vartheta, dV = r^2\sin\vartheta$
$L_x = -i\hbar\left(-\sin\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\cos\varphi\frac{\partial}{\partial\varphi}\right)$, $L_y = -i\hbar\left(-\cos\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\sin\varphi\frac{\partial}{\partial\varphi}\right)$, $L_z = -i\hbar\frac{\partial}{\partial\varphi}$,
$L^2 = -\hbar^2\left(\frac{\partial^2}{\partial\vartheta^2} + \cot\vartheta\frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right)$
Lastne funkcije: $Y_{\ell m}$, lastne vrednosti za L^2 so $\hbar^2\ell(\ell+1)$, za L_z pa $\hbar m$, za $\ell = 0, 1, 2, \ldots$, $m = -\ell, -\ell+1, \ldots, \ell$. Te funkcije so ortonormirane glede na integral po površini sfere.

Atom vodika:
Potencial $V(r) = -\frac{e^2}{4\pi\varepsilon_0 r} = -\frac{\alpha\hbar c}{r}$. Rzstavimo tudi kinetično energijo: $\hat{T} = \frac{\hat{p}^2}{2m} = \frac{1}{2m}(\hat{p}_r + \frac{\hat{L}^2}{\hat{r}^2})$
Lastne funkcije (so ONS) $\Psi_{nlm}(r,\vartheta,\varphi) = R_{n\ell}(r)Y_{\ell m}(\vartheta,\varphi)$, $n = 1, 2, \ldots$, $\ell = 0, \ldots, n-1$, $m_l = -l, \ldots, l$.
Lastne vrednosti: $E_n = -E_{ry}\frac{1}{n^2}$, kjer $E_{ry} = \frac{m_e c^2\alpha^2}{2} = \frac{m_e e^4}{2(4\pi\varepsilon_0)^2\hbar^2} \approx 13.6eV$.
Velja: $\int R_{n'l'}^*(r)R_{nl}(r)r^2dr = \delta_{nn'}\delta_{ll'}$ in $\int Y_{l'm'}^*(\vartheta,\varphi)Y_{lm}(\vartheta,\varphi)d\Omega = \delta_{ll'}\delta_{mm'}$, kjer $d\Omega = d(cos\vartheta)d\varphi$.

Radialni del: $R_{nl}(r) = \sqrt{(\frac{2}{nr_B})^3\frac{(n-l-1)!}{2n(n+l)!}}e^{-\frac{\rho}{2}}\rho^l L_{n-l-1}^{2l+1}(\rho)$, kjer je $\rho = \frac{2r}{nr_B}$.
Bohrov radij $r_B = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = \frac{\hbar c}{m_e c^2\alpha}$
Povprečje potencialne energije: $\langle V\rangle = -\alpha\hbar c\left\langle\frac{1}{r}\right\rangle$, po Bohrovo pa isto, le da velja $r_n = n^2 r_B$ in $\left\langle\frac{1}{r}\right\rangle = \frac{1}{n^2 r_B}$, n je stanje v katerem smo. Izkaže se: $\langle V\rangle_{nlm} = -\frac{\alpha\hbar c}{n^2 r_B}$ za vse n,l,m.
Velja tudi: $\left\langle\frac{1}{r}\right\rangle = \frac{1}{r_B n^2}$, $\left\langle\frac{1}{r^2}\right\rangle = \frac{2}{r_B^2 n^3(2\ell+1)}$, $\left\langle\frac{1}{r^3}\right\rangle = \frac{2}{r_B^3 n^3\ell(\ell+1)(2\ell+1)}$, v osnovnem stanju: $\langle r^p\rangle = \frac{r_B^p}{2^{p+1}}(p+2)!$
Virialni teorem (klasična mehanika): Za potencial oblike $V = \# r^p$ velja $2\langle T\rangle = p\langle V\rangle$. Velja tudi za osnovno stanje vodikovega atoma.
Če računamo $\langle r\rangle$, so koristni "matrični elementi" $\langle i|r|j\rangle = \int R_i^* r R_j r^2 dr$. Velja: $\langle 1|r|1\rangle = \frac{3}{2}r_B, \langle 1|r|2\rangle = \langle 2|r|1\rangle = -\frac{2^5\sqrt{2}}{3^4}r_B \approx -0.5r_B, \langle 2|r|2\rangle = 6r_B$.
Ehrenfestov teorem: Za operator $\mathcal{O}$ velja $\frac{d\langle\mathcal{O}\rangle}{dt} = \frac{1}{i\hbar}\langle[\mathcal{O}, H]\rangle + \left\langle\frac{\partial\mathcal{O}}{\partial t}\right\rangle$. V posebnem to pomeni $\frac{d\langle r\rangle}{dt} = \frac{\langle p\rangle}{m}$, $\frac{d\langle p\rangle}{dt} = -\left\langle\frac{\partial V}{\partial x}\right\rangle$.

Sferični harmoniki: $Y_{lm}(\vartheta,\varphi) = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_{lm}(\cos\vartheta)e^{im\varphi}$.
$\langle l'm'|\mathcal{O}|lm\rangle = \int Y_{l'm'}^*\mathcal{O}Y_{lm}d\Omega$.
$\langle l'm'|\hat{L_x}|lm\rangle = \frac{\hbar}{2}\sqrt{(l\mp m)(l\pm m+1)}\delta_{l'l}\delta_{m',m\pm1}$
$\langle l'm'|\hat{L_y}|lm\rangle = \mp\frac{\hbar}{2}\sqrt{(l\mp m)(l\pm m+1)}\delta_{l'l}\delta_{m',m\pm1}$

$\langle l'm'|\hat{L}_z|lm\rangle = \hbar m_l \delta_{l'l}\delta_{m'm}$
$\langle l'm'|\hat{L}^2|lm\rangle = \hbar^2 l(l+1)\delta_{l'l}\delta_{m'm}$

Spin:
Ko postavimo vodikov atom v magnetno polje, ugotovimo da potrebujemo še spin. Definiramo ga analogno vrtilni količini in označimo s s. Sedaj imamo lastne funkcije: $\psi_{n\ell m_\ell s m_s}$. s je za elektron enak $1/2$, m_s pa teče od $-s$ do s po koraku 1.
Če delec postavimo v magnetno polje, nanj deluje magnetni moment $\hat{\mu} = \frac{e\hbar}{2m\hbar}(g_l\hat{l} + g_s\hat{s}) = \mu_B(g_l\frac{\hat{l}}{\hbar} + g_s\frac{\hat{s}}{\hbar})$, kjer je m masa delca. Za elektron je $g_l = -1$.
Če vzamemo, da magnetno polje deluje le v z-smeri (in je v tej smeri konstantno), sledi $F_z = \langle\mu_z\rangle\frac{\partial B}{\partial z}$, kjer $\mu_z = \frac{e\hbar}{2m}(-1\hat{l_z} + g_s\hat{s_z})$.
s igra isto vlogo kot l, tudi enačbe so enake. Pri danem s je $2s+1$ možnih stanj; $m_s = -s, -s+1, \ldots, s$.
$\left\langle\hat{s^2}\right\rangle = \hbar^2 s(s+1)$, $\langle\hat{s_z}\rangle = \hbar m_s$
Za elektron: $s = \frac{1}{2}$, $g_s = 2$ (slednje je dober približek za vse fermione).
? Hamiltonian popravimo z operatorjem $H_B = -\hat{\mu}B$ in lahko vzamemo da je polje v z smeri, torej $H_{B_z} = -\hat{\mu}_z B_z = \frac{\mu_B B_z}{\hbar}L_z$. Lastne vrednosti $\hat{\mu}^2$ so $\ell(\ell+1)\mu_B$, $\hat{\mu}_z$ pa $m_\ell\mu_B$. Ob tem dodatku postane skupna energija $E_{nm_\ell} = -\frac{E_0}{n^2} + m_\ell\mu_B B$.

LS sklopitev: ($B = 0$) Zaradi interakcije med obema vrtilnima količinama popravimo hamiltonian: $\Delta H_{ls} = \frac{\alpha\hbar c}{2m_e^2c^2}(\hat{\frac{1}{r^3}})\hat{ls}$.
Za izračun lastnih stanj operatorja $\hat{ls}$ je boljša druga baza. (tukaj je $\hat{l} = \hat{L}$) Definiramo skupno vrtilno količino $\hat{j} = \hat{l} + \hat{s}$. velja: $\langle\hat{j}^2\rangle = \hbar j(j+1), \langle\hat{j_z}\rangle = \hbar m_j$, kjer j teče od $|\ell - s|$ do $\ell + s$ po 1. Število m_j kot vedno teče od $-j$ do j. S kvadriranjem j dobimo $\hat{ls} = \frac{1}{2}(\hat{j}^2 - \hat{l}^2 - \hat{s}^2)$. Če je $\ell = 0$, potem ni sklopitve. Lastne vrednosti so $\left\langle\hat{ls}\right\rangle = \frac{1}{2}\hbar^2(j(j+1) - \ell(\ell+1) - s(s+1))$. S to formulo poračunaš $\langle ls\rangle$ za vse možne kombinacije $n, l, j (s = 1/2)$ in nato vsakega posebej vstaviš v ΔE_{ls}.
Pretvorba: $\psi_{n\ell m_\ell s m_s} = \sum c^{\ell s j m_j}_{\ell m_\ell s m_s}\psi_{n\ell s j m_j}$. Koeficiente preberemo iz tabele (pozor, v tabeli so vsi skvadrirani!!). Verjetnost, da neko stanje izmerimo, je ustrezni koeficient na kvadrat.

Močno magnetno polje: (ne rabimo iti v novo bazo) Razcep $\Delta E = \mu_B(m_\ell + 2m_s)B_z$. $B > 1/6T$, da smo c tem približku. V osnovnem stanju: $\Delta E = \pm\mu_B B$.

Šibko magnetno polje: (rabimo novo bazo) Razcep $\Delta E = \langle H_B\rangle = \frac{\mu_B}{\hbar}B_z(\langle l_z\rangle + 2\langle s_z\rangle)$.
$\langle s_z\rangle = \frac{\langle j_z\rangle\langle sj\rangle}{\langle j^2\rangle}$, $\langle sj\rangle = \frac{1}{2}(j^2 + s^2 - l^2)$, $\langle l_z\rangle = \frac{\langle j_z\rangle\langle lj\rangle}{\langle j^2\rangle} = \frac{\langle j_z\rangle\left\langle j^2 - sj\right\rangle}{\langle j^2\rangle}$
$\Delta E = \mu_B B_z m_j g_j$, kjer $g_j = 1 + \frac{\left\langle j^2 + s^2 - l^2\right\rangle}{2\langle j^2\rangle} = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}$. To poračunaš za vse možne n,l,j.

Perturbacije: $\hat{H} = \hat{H}_0 + \varepsilon\hat{H}_1$
$|n\rangle$ n-to stanje H, $|n_0\rangle$ n-to stanje od H_0, $|n_i\rangle$ n-to stanje v i-tem redu preturbacije; $H|n\rangle = E_n|n\rangle$
$|n\rangle = |n_0\rangle + \varepsilon|n_1\rangle + \varepsilon^2|n_2\rangle + \ldots, E_n = E_{n0} + \varepsilon E_{n1} + \varepsilon^2 E_{n2} + \ldots$
POPRAVEK 1. REDA: $E_{n1} = \langle n_0|\hat{H}_1|n_0\rangle$, $|n_1\rangle = \sum_{m\neq n}\frac{\langle m_0|\hat{H}_1|n_0\rangle}{E_{n0} - E_{m0}}|m_0\rangle$
POPRAVEK 2. REDA: $E_{n2} = \sum_{m\neq n}\frac{|\langle m_0|\hat{H}_1|n_0\rangle|^2}{E_{n0} - E_{m0}}$ (vedno pride < 0)

Neharmonski operator: V vsakem primeru uvedemo $a = \frac{1}{\sqrt{2}}(\frac{x}{x_0} + \frac{i}{\hbar}x_0 p), a^+ = \frac{1}{\sqrt{2}}(\frac{x}{x_0} - \frac{i}{\hbar}x_0 p), n = a^+a, n+1 = aa^+$. Velja $[x,p] = i\hbar, [a, a^+] = 1, \frac{x}{x_0} = \frac{a + a^+}{\sqrt{2}}$.
$a|n\rangle = \sqrt{n}|n-1\rangle, a^+|n\rangle = \sqrt{n+1}|n+1\rangle, \hat{n}|n\rangle = n|n\rangle$
$H_0 = \hbar\omega(\hat{n} + 1/2)$
Če je $H_1 = \varepsilon_4\hbar\omega(\frac{x}{x_0})^4 = \varepsilon_4\hbar\omega\frac{1}{\sqrt{2}^4}(\hat{a} + \hat{a^+})^4$, dobimo $E_{n1} = \frac{3\varepsilon_4\hbar\omega}{2}(n^2 + n + \frac{1}{2})$ (ostanejo le členi, kjer je enako število a in a^+), to je dober približek, dokler $E_{n0} > E_{n1}$.
Če $H_1 = \varepsilon_3\hbar\omega(\frac{x}{x_0})^3 = \varepsilon_3\hbar\omega\frac{1}{\sqrt{2}^3}(\hat{a} + \hat{a^+})^3$, je $E_{n1} = 0$ in $E_{n2} = -\frac{\hbar\omega\varepsilon_3^2}{8}(30(n+1)n + 11)$ (smiselni m-ji so le $n-3, n-1, n+1, n+3$, ker a in a^+ ravno dvigata/spuščata stanja).

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