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Kvantron. 8

7/10-08, FL 72

13¹⁵-15⁰⁰

XII. 7, 8, 9, 10

XIII. 2, 4, 7

XII.7

Natrium atomen ~ en el. atom

$$\hat{H} = \hat{H}_0 + \frac{\xi(r)}{\hbar^2} \hat{L} \cdot \hat{S}$$

particentral fält Ham.

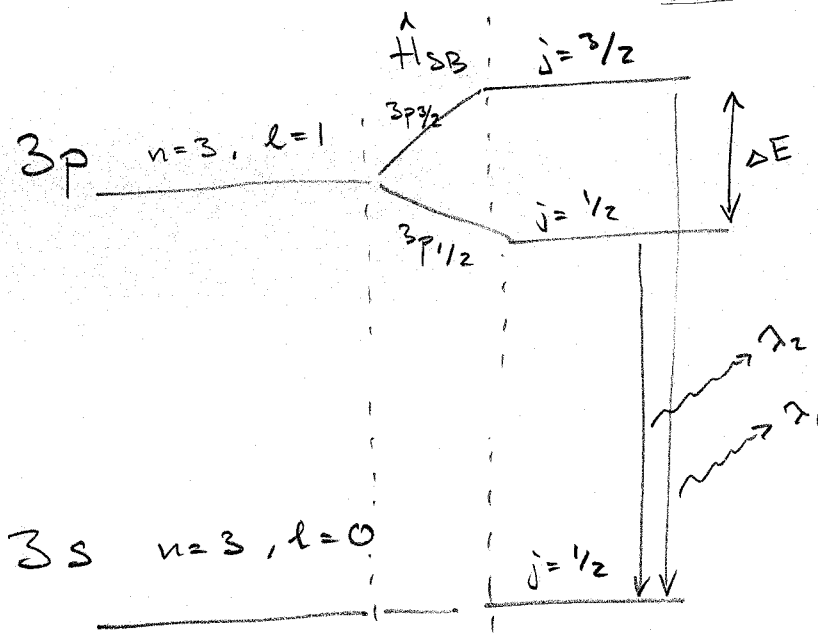
Spin-Balkoppling ger finstruktur i spektra!

3p → 3s övergång delas i två komponenter.

Gula D-dubletten: $\lambda_1 = 5889.95 \text{ \AA}$
 $\lambda_2 = 5895.92 \text{ \AA}$

Beräkna väntevärdet av $\xi(r)$ i 3p-tillståndet. $\Rightarrow \langle 3p | \xi(r) | 3p \rangle = \xi_{31}$
 (spinorbital) i eV

Spinorbalkoppling: Goda kvanttal n, l, j, m_j
 $j = l \pm 1/2$ för en el. $E_{nlj} = E_{nl}^{(0)} + \frac{\hbar^2}{2} [j(j+1) - l(l+1) - s(s+1)] \xi_{nl}$



Övergångsregler:
 $\Delta l = \pm 1$
 $\Delta j = 0, \pm 1$
 Ok i detta fall!

ej $j = -1/2$ ty längd på tot. magn. mom. (12.34 komponenter)

$$\Delta E = E_{\lambda_1} - E_{\lambda_2} = hc \left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2} \right) = E_{31\frac{3}{2}} - E_{31\frac{1}{2}} =$$

$$= \frac{\hbar^2}{2} \xi_{31} \left[\frac{3}{2} \left(1 + \frac{3}{2} \right) - \frac{1}{2} \left(1 + \frac{1}{2} \right) \right] = \frac{3\hbar^2}{2} \xi_{31}$$

$$\frac{3 \cdot 5}{4} - \frac{3}{4} = \frac{12}{4} = 3$$

$$\frac{\hbar^2}{2} \xi_{31} = \frac{2}{3} hc \left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2} \right) \approx 1.4 \text{ meV} \quad \text{energi skala för SB koppling.}$$

XII.8 Lagg på magnetfält! $B = B\hat{z}$

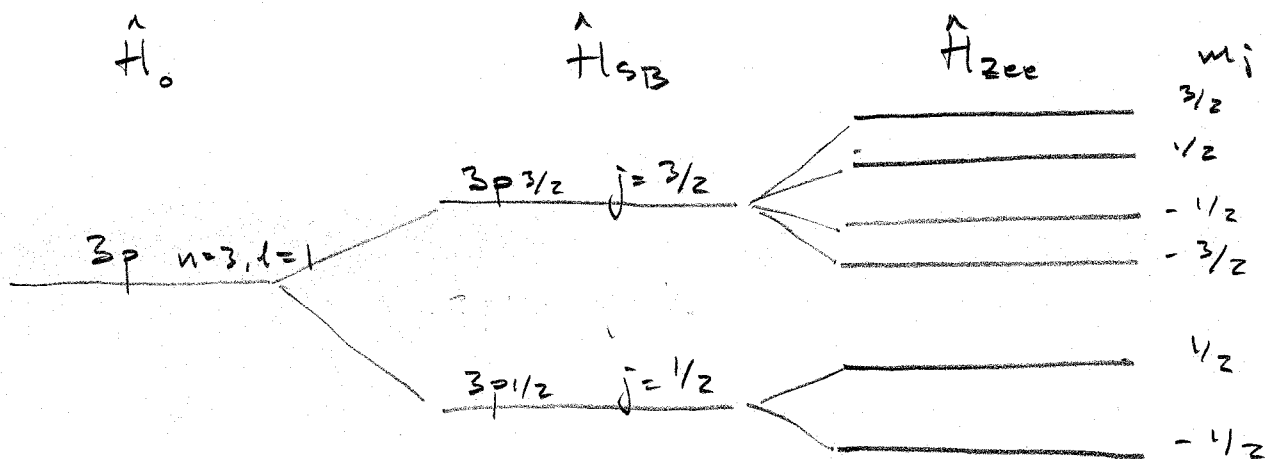
Änge hur natriumdubletten uppsplittas:

$$\text{Nu: } \hat{H} = \hat{H}_0 + \underbrace{\frac{\xi(r)}{\hbar^2} \hat{L} \cdot \hat{S}}_{\hat{H}_{SB}} + \underbrace{\frac{\mu_B B}{\hbar} (\hat{L}_z + 2\hat{S}_z)}_{\text{Zeeman eff.}}$$

a) Energier: $E_{nljm_j} = E_{nlj} + g_j \mu_B B m_j$

g_j Landé's g-faktor: $g_j = 1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)}$

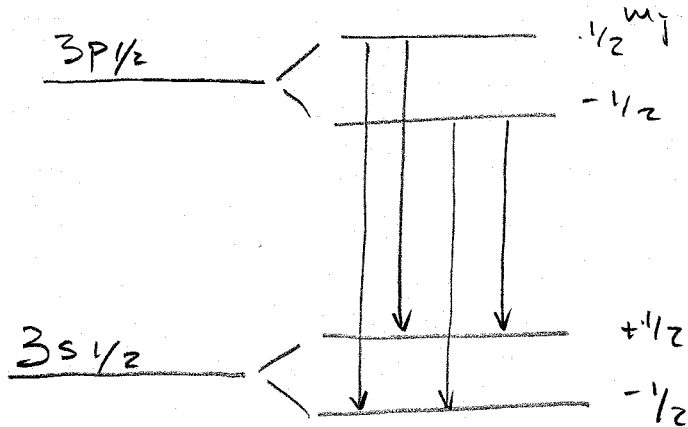
$j = l \pm 1/2$; $m_j = -j, -j+1, \dots, j-1, j$



XII. 8 forts / Tillätna över g.

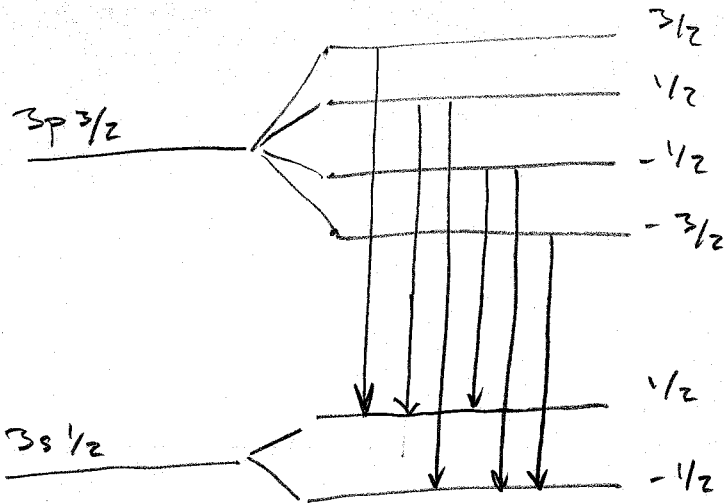
$$\left\{ \begin{array}{l} \Delta l = \pm 1 \\ \Delta j = 0, \pm 1 \\ \Delta m_j = 0, \pm 1 \end{array} \right.$$

Första löpjen i Dubletten:



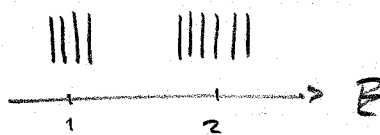
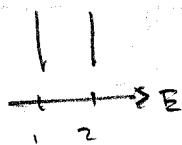
$\Rightarrow 3P_{1/2} \rightarrow 3S_{1/2}$
 splittras i 4 delar

Andra löpjen i Dubletten m_j

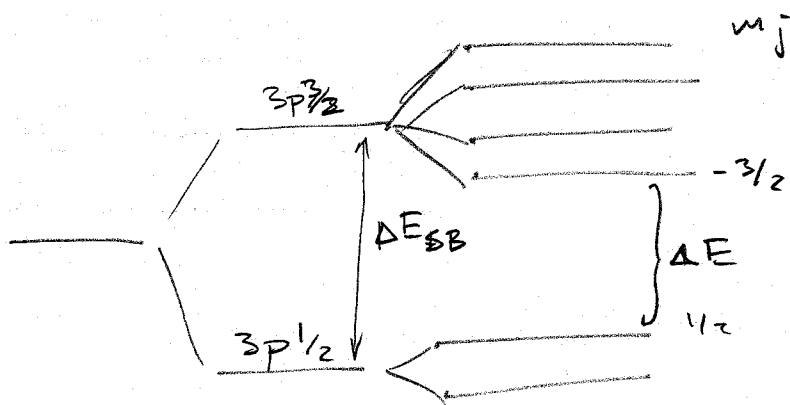


$\Rightarrow 3P_{3/2} \rightarrow 3S_{1/2}$
 splittras i 6 delar

Dvs. 5896\AA delas i 4 & 5890\AA i 6 delar



XII.8 / b) För vilket magnetfält B sammanfaller
 lägsta $3p_{3/2}$ nivå med högsta $3p_{1/2}$



Sammanfall. \Rightarrow
 $\Delta E = 0$

$$\Delta E = \Delta E_{SB} + g_{3/2} \mu_B B \left(-\frac{3}{2}\right) - g_{1/2} \mu_B B \left(\frac{1}{2}\right)$$

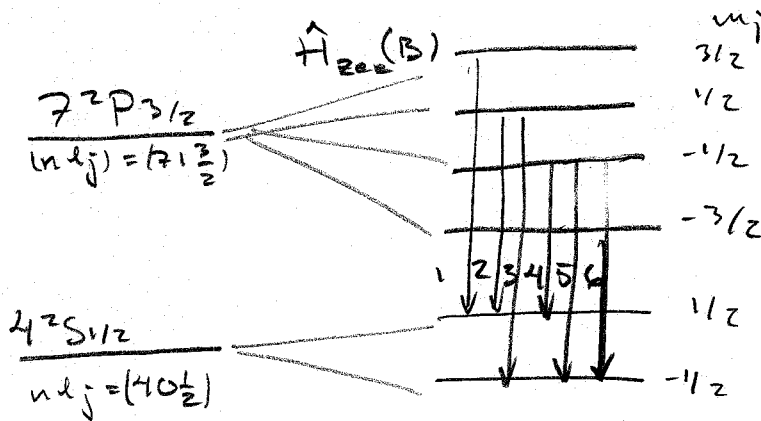
$$g_{3/2} = \dots = \frac{4}{3} \quad ; \quad g_{1/2} = \dots = \frac{2}{3}$$

$$\Rightarrow \Delta E = hc \left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2} \right) - \mu_B B \underbrace{\left(\frac{4}{3} \frac{3}{2} + \frac{2}{3} \frac{1}{2} \right)}_{7/3} = 0$$

$$\Rightarrow B = hc \left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2} \right) \frac{3}{7 \mu_B} \approx \underline{\underline{15,8 \text{ T}}}$$

XII.9 / Kaliumns P-serie har en spektrallinje motsv. överg. $7^2P_{3/2} - 4^2S_{1/2}$
 m. $\lambda = 3217 \text{ \AA}$.

Lande's g-fakt. är $\frac{4}{3}$ för $P_{3/2}$ & 2 för $S_{1/2}$
 Ber uppsplutningen av linjen i ett yttre magnetfält. $B = 2.14 \text{ T}$



Söker energiskilnaden ΔE mellan $(B=0)$ $7^2P_{3/2} \rightarrow 4^2S_{1/2}$ överg. & 1, ..., 6 uppspluttrade överg.

$$\Delta E = \delta E_{3/2 m_j} - \delta E_{1/2 m_j}$$

$$\delta E_{j m_j} = g_j \mu_B B m_j \Rightarrow \frac{\delta E}{\mu_B B} = g_j m_j$$

m_j	g_j	$\frac{\delta E_{j m_j}}{\mu_B B}$
$j = 3/2$		
3/2	4/3	2
1/2		2/3
-1/2		-2/3
-3/2		-2
$j = 1/2$		
1/2	2	1
-1/2		-1

$$\Rightarrow \frac{\Delta E_1}{\mu_B B} = 2 - 1 = 1$$

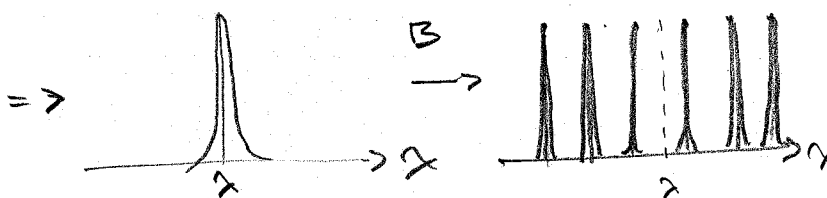
$$\frac{\Delta E_2}{\mu_B B} = \frac{2}{3} - 1 = -\frac{1}{3}$$

$$\frac{\Delta E_3}{\mu_B B} = \frac{2}{3} + 1 = \frac{5}{3}$$

$$\frac{\Delta E_4}{\mu_B B} = -\frac{2}{3} - 1 = -\frac{5}{3}$$

$$\frac{\Delta E_5}{\mu_B B} = -\frac{2}{3} + 1 = \frac{1}{3}$$

$$\frac{\Delta E_6}{\mu_B B} = -2 + 1 = -1$$



XII, 10/

Positronium.

$$S_{e^-} = S_{e^+} = \frac{1}{2}$$

$$H = H_0 + \frac{A}{\hbar^2} \hat{S}_1 \cdot \hat{S}_2$$

Koppling mellan spinnen hos e^- & e^+

Grundtillstånd splittras i

1S_0 & 3S_1

S_{tot} är totala spinnet.

De två tillstå. motsv.

$$1 = 2S_{tot} + 1$$

$$S_{tot} = 0$$

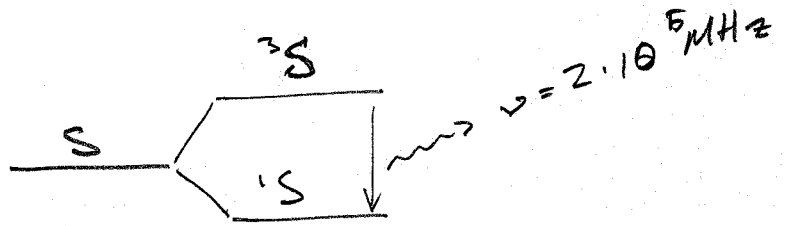
$$e = 0$$

$$\Rightarrow 3 = 2S_{tot} + 1$$

$$S_{tot} = 1$$

$$S_{tot} = 0 : \uparrow\downarrow$$

$$S_{tot} = 1 : \uparrow\uparrow$$



Ber: A

$$\Delta E = h\nu = \langle \frac{A}{\hbar^2} \hat{S}_1 \cdot \hat{S}_2 \rangle_{3S} - \langle \frac{A}{\hbar^2} \hat{S}_1 \cdot \hat{S}_2 \rangle_{1S}$$

$$\langle \hat{S}_1 \cdot \hat{S}_2 \rangle = \text{konstruera.} = \langle \frac{1}{2} [(\hat{S}_1 + \hat{S}_2)^2 - \hat{S}_1^2 - \hat{S}_2^2] \rangle$$

$$\hat{S}_1^2 \text{ \& \ } \hat{S}_2^2 \text{ har egenv. } \langle \hat{S}_i^2 \rangle = \hbar^2 s_i(s_i + 1) = \frac{3\hbar^2}{4}$$

(samma för båda tillst.)

$$s_i = \frac{1}{2} = S_{e^-} = S_{e^+}$$

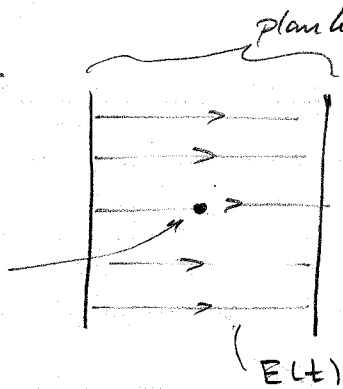
$$\langle (\hat{S}_1 + \hat{S}_2)^2 \rangle = \langle \hat{S}_{tot}^2 \rangle = \hbar^2 S_{tot}(S_{tot} + 1) = \begin{cases} 0, & 1S \\ 2\hbar^2, & 3S \end{cases}$$

$$\Rightarrow \Delta E = h\nu = \frac{A}{\hbar^2} \frac{1}{2} (2\hbar^2 - 0) = A!$$

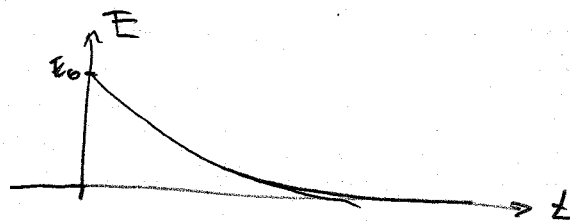
$$A = h\nu \approx 0,8 \text{ meV}$$

XIII. 2 /

Väteatom
i g.s. 1s
 $t=0$



$$E(t) = \begin{cases} 0, & t < 0 \\ E_0 e^{-t/\tau}, & t \geq 0 \end{cases}$$



Ber: $P(Z_s)$ för $t \rightarrow \infty$ m. lägsta ordns störteori.

$$H = H_0 + \hat{V}(t) \quad ; \quad H_0 \psi_n = E_n \psi_n$$

↑
störteori

$$\Rightarrow \text{Generell lösning: } \psi(t) = \sum_{n=0}^{\infty} c_n(t) \psi_n(r) e^{-i/\hbar E_n t}$$

Vet $t=0$: $\psi = \psi_{100} \Rightarrow |c_{100}|^2 = 1$ läst $c_s = c_{100}$

Fermis gyllene regel:

$$c_k(t) = \delta_{ks} - \frac{i}{\hbar} \int_0^t \langle k | V(t') | s \rangle e^{i\omega_{ks} t'} dt'$$

$$\omega_{ks} = \frac{1}{\hbar} (E_k - E_s)$$

Nu $s=100, k=200$ (Z_s)

$$\hat{V}(t) ? \quad E = E \hat{z} ; \quad F = e E \hat{z} = -\nabla \hat{V}$$

$$\Rightarrow \hat{V} = -\hat{z} \int F_z dz = -e E(t) z \hat{z}$$

↑ konst.

Obs! $l=0 \Rightarrow$ inget θ, φ var.

$$\langle 200s | \hat{V}(t) | 100s \rangle = \int dV \psi_{200}^*(r) e E(t) z \psi_{100}(r)$$

$$= e E(t) \int_0^{2\pi} d\varphi \int_0^\pi \cos\theta \sin\theta d\theta \int_0^\infty \psi_{200}^*(r) \psi_{100}(r) r^2 dr$$

$$= \int_0^\pi \frac{1}{2} \sin 2\theta d\theta = 0$$

Hel period!

$$\Rightarrow |c_{200}(t)|^2 = 0 = P(Z_s)_{t \rightarrow \infty}$$

E-fältet kan inte excitera atomer!
Eftersom fältet är homogent - just stora överlapp

XIII. 4 / Gyllene regeln: Samordligheten
 för dipolöverg. best. av $\langle k | e | \pi \rangle$

Visa att: $\langle k | e | \pi \rangle = i\mu\omega_{ks} \langle k | e | \pi \rangle$
elektriskt dipolmoment

Lösning: $[\hat{H}_0, \pi] = \left[\frac{p^2}{2\mu} + V(r), \pi \right] =$

$= \frac{1}{2\mu} [p^2, \pi] = \frac{1}{2\mu} [p_x^2 + p_y^2 + p_z^2, x\hat{x} + y\hat{y} + z\hat{z}] =$
↑ enhetsvekt.

$= \frac{1}{2\mu} \left([p_x^2, x]\hat{x} + [p_y^2, y]\hat{y} + [p_z^2, z]\hat{z} \right) =$

$= \frac{1}{2\mu} \left([p_x^2, x] = p_x [p_x, x] + [p_x, x] p_x = -2i\hbar p_x \right) =$

$= \frac{-2i\hbar}{2\mu} (p_x\hat{x} + p_y\hat{y} + p_z\hat{z}) = -\frac{i\hbar}{\mu} p$

$\Rightarrow \underline{p = \frac{i\mu}{\hbar} [H_0, \pi]}$

Ans. $\langle k | e | \pi \rangle = \frac{i\mu e}{\hbar} \langle k | [H_0, \pi] | s \rangle =$

$= \frac{i\mu e}{\hbar} \left(\underbrace{\langle k | H_0 | \pi \rangle}_{= E_k \langle k |} - \langle k | \pi \underbrace{H_0 | s \rangle}_{= E_s | s \rangle} \right) =$

$= \frac{i\mu e}{\hbar} (E_k \langle k | \pi \rangle - E_s \langle k | \pi \rangle) =$

$= i\mu \underbrace{\frac{E_k - E_s}{\hbar}}_{= \omega_{ks}} \langle k | e | \pi \rangle = i\mu\omega_{ks} \langle k | e | \pi \rangle$

ok!

XII.7 / 1D Harmon osc. med massa m
 vinkel frekv. ω & laddning q i elektriskt
 fält: $E = E_0 \cos \nu t$

Ber: överg. sannolikheten för överg.

a) $n: 0 \rightarrow 1$ b) $n: 1 \rightarrow 2$ c) $n: 0 \rightarrow 2$

Fermi:

$$c_{i \rightarrow f}(t) = -\frac{i}{\hbar} \int_0^t \langle f | V(t') | i \rangle e^{i\omega_{fi} t'} dt'$$

↑ initial & final state

$$P(i \rightarrow f) = |c_{i \rightarrow f}|^2$$

Ber stor. V :

$$E = E_0 \cos \nu t \Rightarrow F = q E_0 \cos \nu t, \quad F = -\nabla V = -\frac{\partial}{\partial x} V$$

$$\underline{V = -q E_0 x \cos \nu t}$$

Tillståndes vågfunk.

jämn $\psi_0 = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}\alpha^2 x^2} \quad (\alpha = \sqrt{\frac{m\omega}{\hbar}})$

udda $\psi_1 = \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} 2\alpha x e^{-\frac{1}{2}\alpha^2 x^2}$

jämn. $\psi_2 = \left(\frac{\alpha}{8\sqrt{\pi}}\right)^{1/2} (4\alpha^2 x^2 - 2) e^{-\frac{1}{2}\alpha^2 x^2}$

Vilka matris el. kommer vara $\neq 0$?

$$\langle f | V(t') | i \rangle = \int_{-\infty}^{\infty} \psi_f^* V(t') \psi_i dx = -q E_0 \cos \nu t \cdot \int_{-\infty}^{\infty} \psi_f^* x \psi_i dx$$

$\int_{-\infty}^{\infty} \psi_f^* x \psi_i dx$
 om udda = 0!

a) $\langle 1 | V | 0 \rangle \neq 0 \Rightarrow |c_{0 \rightarrow 1}|^2 \neq 0$

b) $\langle 2 | V | 1 \rangle \neq 0 \Rightarrow |c_{1 \rightarrow 2}|^2 \neq 0$

c) $\langle 2 | V | 0 \rangle = 0 \Rightarrow |c_{0 \rightarrow 2}|^2 = 0!$