

BÖLÜM 17

REEL HİDROJEN ATOMU

hidrojen benzeri atomların tartışılması

$$H_0 = \frac{\vec{p}^2}{2\mu} - \frac{Ze^2}{r}$$

Hamiltonienini almıştık. Proton hareketli yaklaşımı -
Çizimden relativistik etkileri ve spin etkileri ile ilgili
yönelimimiz.

$$K = \frac{\vec{p}_e^2}{2m_e} + \frac{\vec{p}_p^2}{2m_p} = \frac{1}{2} \vec{p}^2 \left(\frac{1}{m_e} + \frac{1}{m_p} \right) \approx \frac{\vec{p}^2}{2\mu}$$

$$\vec{p} = \vec{p}_e = -\vec{p}_p \text{ akm. (K.M. 'de)}$$

$$\mu/m_e \approx 1 - \frac{m_e}{m_p} \approx 1 - 5.4 \times 10^{-4}$$

protonun elektronu göre daha ağır olduğunu ve hareket
etmediğini varsayalım.

RELATIVİSTİK KINETİK ENERJİ ETKİLERİ

Elektronun K.E.'si

$$K = [\vec{p}^2 c^2 + m_e^2 c^4]^{1/2} - m_e c^2$$

$$= m_e c^2 \left[1 + \frac{\vec{p}^2}{m_e^2 c^2} \right]^{1/2} - m_e c^2$$

$$K \approx m_e c^2 \left[1 + \frac{1}{2} \frac{\vec{p}^2}{m_e^2 c^2} - \frac{1}{8} \left(\frac{\vec{p}^2}{m_e^2 c^2} \right)^2 + \dots \right] - m_e c^2$$

$$= \frac{\vec{p}^2}{2m_e} - \frac{1}{8} \frac{(\vec{p}^2)^2}{m_e^3 c^2} + \dots$$

$$H_1 = - \frac{1}{8} \frac{(\vec{p}^2)^2}{m_e^3 c^2} \quad \text{perturbasyon}$$

independen; hâle etirine büyük
hâle.

Spin-Yönü etirilmesi

Elektron hareketi sonucu ile doğru
magnetik alan

$$\vec{B} \sim \frac{\vec{v} \times \vec{E}}{c} \rightarrow \text{bu } \vec{S} \text{ ile etirilir}$$

$$\vec{M} = - \frac{e \hbar}{2m_e c} \vec{S}$$

$$-\vec{A} \cdot \vec{B} = \frac{e\hbar}{2mc} \vec{S} \cdot \vec{B} = -\frac{e\hbar}{2mc} \vec{S} \cdot \frac{\vec{v} \times \vec{E}}{c}$$

$$= +\frac{e}{mc^2} \vec{S} \cdot \vec{v} \times \vec{\nabla} \phi$$

$$= \frac{e}{(mc)^2} \vec{S} \cdot \underbrace{\vec{p} \times \vec{r}}_{-\vec{L}} \frac{1}{r} \frac{d\phi}{dr}$$

$$= -\frac{e}{mc^2} \vec{S} \cdot \vec{L} \frac{1}{r} \frac{d\phi}{dr}$$

$$H_2 = -\frac{1}{2mc^2} \vec{S} \cdot \vec{L} \frac{1}{r} \frac{d[e\phi(r)]}{dr}$$

Thomas kayan. (elektron dairesel hareketi için)

Şimdi H_2 'nin benzeri atomların spektrumuna H_1 'ne H_1 'in etkilerini 1. mertebe pertürbasyon teorisi ile hesaplayalım.

$$H_1 = -\frac{1}{2} \frac{(\vec{p})^2}{mc^2} = -\frac{1}{2mc^2} \left(\frac{\vec{p}}{2mc} \right)^2$$

$$= -\frac{1}{2mc^2} \left(H_0 + \frac{Ze^2}{r} \right)^2 = -\frac{1}{2mc^2} \left(H_0 + \frac{Ze^2}{r} \right) \left(H_0 + \frac{Ze^2}{r} \right)$$

4

$$\langle \phi_{\text{new}} | H_1 | \phi_{\text{new}} \rangle = -\frac{1}{2m\tilde{c}^2} \langle \phi_{\text{new}} | \left(\nabla^2 + \frac{ze^{\sim}}{r} \right) \left(\nabla^2 + \frac{ze^{\sim}}{r} \right) | \phi_{\text{new}} \rangle$$

$$= -\frac{1}{2m\tilde{c}^2} \langle \phi_{\text{new}} | \left[\nabla^2 + (ze^{\sim}) \frac{1}{r^2} + ze^{\sim} \left(\nabla^2 \frac{1}{r} + \frac{1}{r} \nabla^2 \right) \right] | \phi_{\text{new}} \rangle$$

$$= -\frac{1}{2m\tilde{c}^2} \left[E_n^2 + (ze^{\sim}) \left\langle \frac{1}{r^2} \right\rangle + 2 E_n ze^{\sim} \left\langle \frac{1}{r} \right\rangle \right]$$

$$= -\frac{1}{2m\tilde{c}^2} \left\{ \left[\frac{m\tilde{c}^2 (Z\alpha)^2}{2n^2} \right]^2 - 2 ze^{\sim} \frac{m\tilde{c}^2 (Z\alpha)^2}{2n^2} \frac{Z}{a_0 n^2} + \frac{(ze^{\sim})^2}{n^3} \frac{Z}{a_0 n^2 (l+1/2)} \right\}$$

$$= -\frac{1}{2} m\tilde{c}^2 (Z\alpha)^2 \left\{ \frac{(Z\alpha)^2}{n^3 (l+1/2)} - \frac{2 (Z\alpha)^2}{4n^4} \right\}$$

$$\phi(r) = \frac{ze}{r}$$

$$H_2 = -\frac{1}{2m\tilde{c}^2} \vec{S} \cdot \vec{L} \frac{1}{r} \frac{d\phi}{dr}$$

$$= + \frac{ze^{\sim}}{2m\tilde{c}^2} \vec{S} \cdot \vec{L} \frac{1}{r^2}$$

$$\vec{J} = \vec{L} + \vec{S}$$

$$\vec{S} \cdot \vec{L} = \frac{1}{2} (\vec{J}^2 - \vec{L}^2 - \vec{S}^2)$$

$$\vec{S} \cdot \vec{L} \psi_{j=l+1/2, m_j=m+1/2} = \frac{1}{2} (\vec{J}^2 - \vec{L}^2 - \vec{S}^2) \psi$$

$$= \frac{1}{2} \hbar^2 \left[(l+1/2)(l+3/2) - l(l+1) - \frac{3}{4} \right] \psi$$

$$= \frac{\hbar^2}{2} l \psi$$

$$\vec{S} \cdot \vec{L} \psi_{j=l-1/2, m_j=m+1/2} = \frac{\hbar^2}{2} \left[(l-1/2)(l+1/2) - l(l+1) - \frac{3}{4} \right] \psi$$

$$= -\frac{\hbar^2}{2} (l+1) \psi$$

$$\langle \psi_{j,m;l} | H_z | \psi_{j,m;l} \rangle = \frac{2e\hbar}{2m_e c} \frac{\hbar^2}{2} \left\{ \begin{matrix} l \\ -l-1 \end{matrix} \right\}$$

$$\times \int_0^\infty dr r^2 R_{nl}^2 \frac{1}{r}$$

$$\frac{2^3}{a_0^3} \frac{1}{n^3 (l+1/2)(l+1)} \quad l \neq 0$$

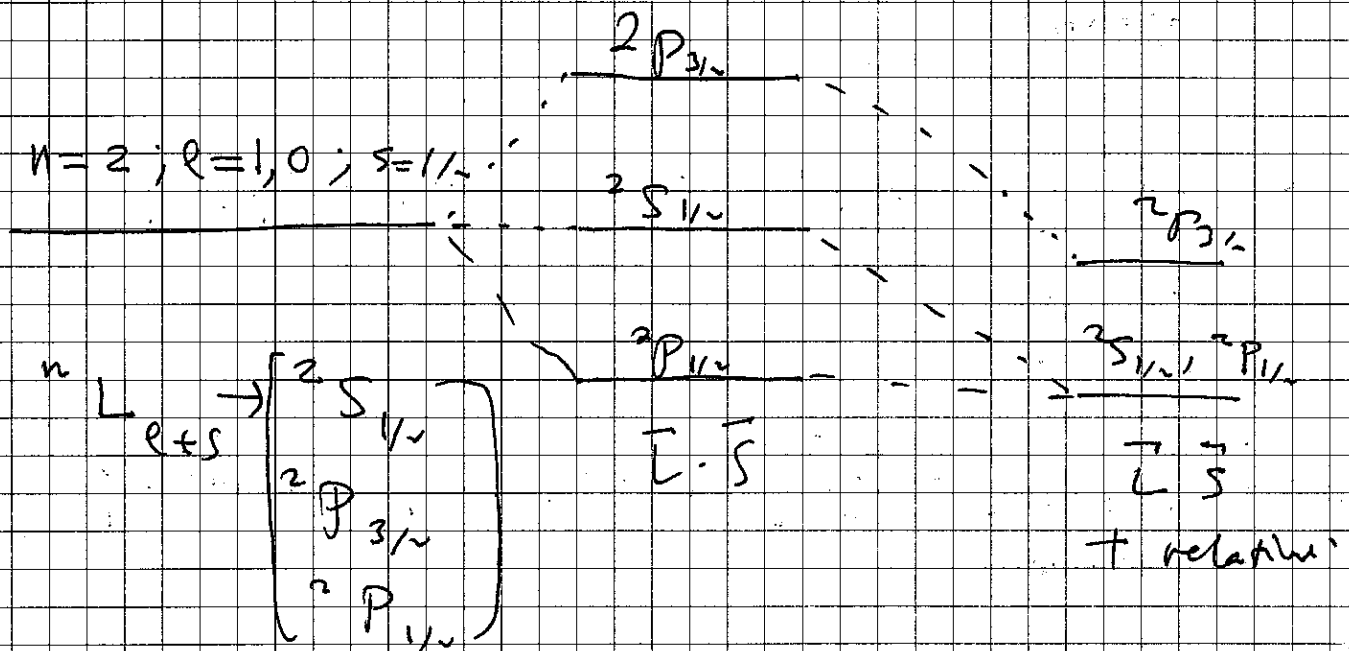
$$a_0 = \hbar / \mu c \alpha$$

$$\Delta E_z = \frac{1}{4} m_e c^2 (2\alpha)^4 \frac{1}{n^3 l(l+1/2)(l+1)} \left\{ \begin{matrix} l \\ -l-1 \end{matrix} \right\} \quad l \neq 0$$

$$\int \pi_1 \sim \pi_2$$

$$\Delta E = -\frac{1}{4} m_e c^2 (2\alpha)^4 \frac{1}{n^3} \left[\frac{1}{j+1/2} - \frac{3}{4n} \right] \quad l = j \pm 1/2$$

BS $K(l=0) \Rightarrow$ Dirac result.



Anomalous Zeeman Effect

$$H_0 = \frac{\vec{p}^2}{2m} - \frac{Ze^2}{r} + \frac{1}{2m\epsilon^2 c^2} \frac{Ze^2}{r^3} \vec{L} \cdot \vec{S}$$

$$H_1 = \frac{e}{2m\epsilon c} (\vec{L} + 2\vec{S}) \cdot \vec{B}$$

gyromagnetic ratio $g = 2$

$$\vec{\mu} = -\frac{e\hbar}{2m\epsilon c} \vec{S}$$

$$\vec{B} = B \hat{z}$$

$$\langle \phi_{jmje} | \frac{eB}{2m\epsilon c} (L_z + 2S_z) | \phi_{jmje} \rangle$$

$$= \langle \frac{eB}{2m\epsilon c} (J_z + S_z) \rangle = \frac{eB}{2m\epsilon c} (\hbar m_j + \langle S_z \rangle)$$

$$j = l + 1/2$$

$$\left\langle \sqrt{\frac{l+m+1}{2l+1}} Y_{lm} X_+ + \sqrt{\frac{l-m}{2l+1}} Y_{lm+1} X_- \right| S_z$$

$$\left| \sqrt{\frac{l+m+1}{2l+1}} Y_{lm} X_+ + \sqrt{\frac{l-m}{2l+1}} Y_{lm+1} X_- \right\rangle$$

$$= \frac{\hbar}{2} \left(\frac{l+m+1}{2l+1} - \frac{l-m}{2l+1} \right) = \frac{\hbar}{2} \frac{2m+1}{2l+1} = \frac{\hbar m_j}{2l+1}$$

○

$$j = l - 1/2$$

$$\left\langle \sqrt{\frac{l-m}{2l+1}} Y_{lm} X_+ - \sqrt{\frac{l+m+1}{2l+1}} Y_{lm+1} X_- \right| S_z$$

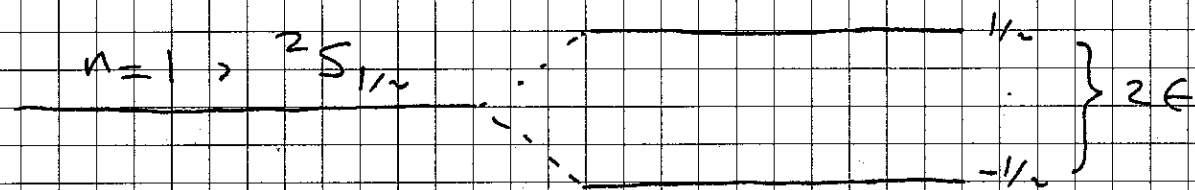
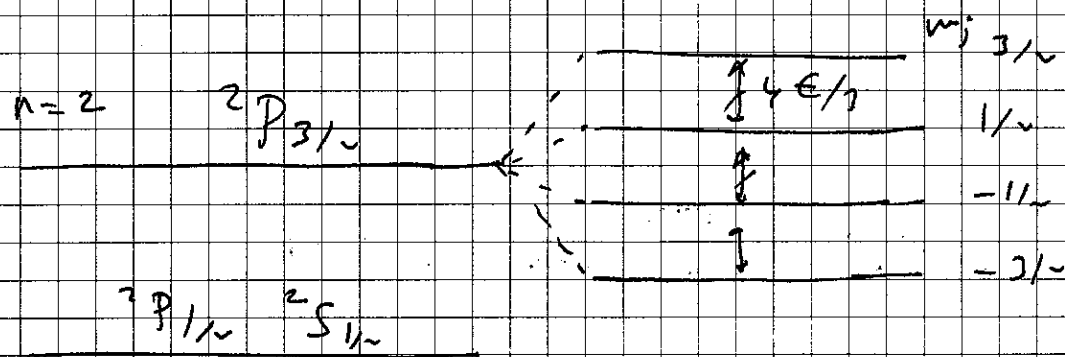
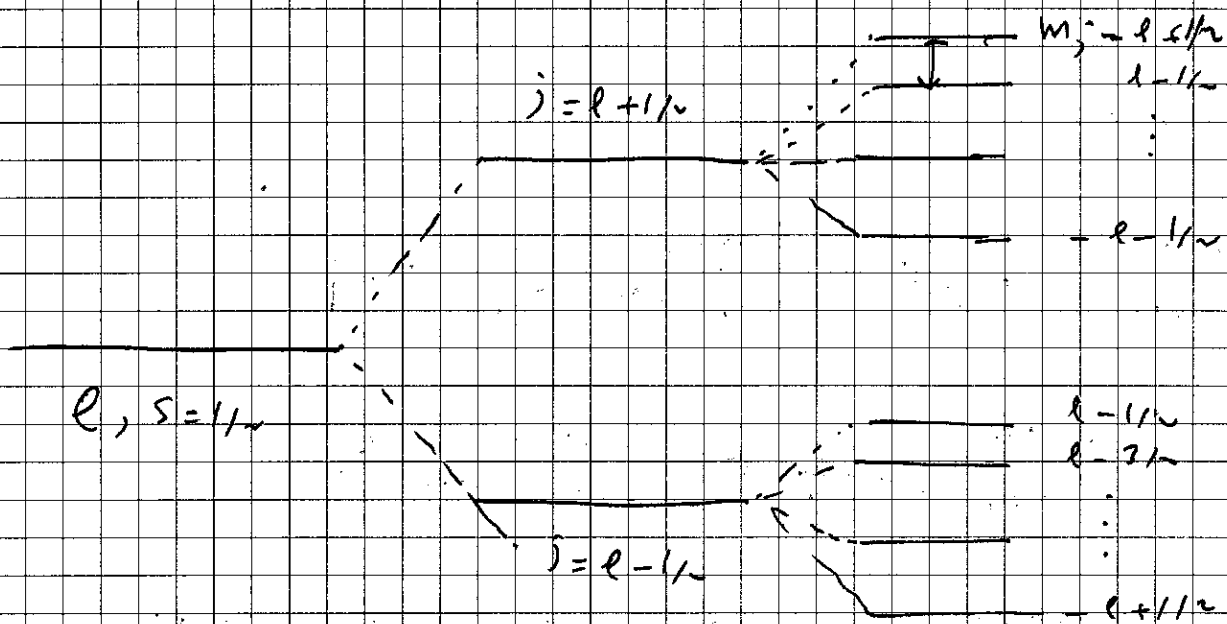
$$\left| \sqrt{\frac{l-m}{2l+1}} Y_{lm} X_+ - \sqrt{\frac{l+m+1}{2l+1}} Y_{lm+1} X_- \right\rangle$$

$$= \frac{\hbar}{2} \left(\frac{l-m}{2l+1} - \frac{l+m+1}{2l+1} \right) = -\frac{\hbar}{2} \frac{2m+1}{2l+1} = -\frac{\hbar m_j}{2l+1}$$

○

$$\Delta E = \frac{e \hbar B}{2 m_e c} m_j \left(1 \pm \frac{1}{2l+1} \right) \quad j = l \pm 1/2$$

$$\Delta m_j = \pm 1, 0$$



Tarixima herçolun içi ayn deñirib, karmel zeenon olay
 içi elde ettiğimize içi sığışi elde edemeyiz. Örneğin $n=2$ içi
 $2p_{3/2}$ 4 qışide ayılab $2p_{1/2}$ den içi heri deñi sığış. Buñ olan
 karmeliñ de ($\bar{L}-\bar{S}$ içi heri edebiler) barıştıe sığışılmalı capilman,
 karmeliñ deñi sığışılmalı karmeliñ deñi sığışılmalı.

L_z ve S_z 'nin özeğelerini m_l ve m_s olarak adlandırarak μ_B 'in çekilen değeri ($\vec{B} = B\hat{z}$)

$$\langle \mu_B \rangle = \frac{e\hbar B}{2mc} (m_l + 2m_s)$$

Böylece $n=2$, $l=1$; $m_l = \pm 1, 0$ ve $m_s = \pm 1/2$ değerlerinde karşılık gelen 5 çizgiye ayrılır.

ASIRI İNCE YAPIL

○ $\vec{L}$, $\vec{S}$ kuantum spin olduğun ince yapılı olan bir cisminin magnetik dipol mom.'i tarafından ilave edilen magnetik alandan dolayı daimi bir Zeeman yarılmazı olan çok ince bir yapıya ince yapılı da vardır. $\vec{I}$ cisminin spin olan magnetik dipol mom. op.'i

$$\vec{\mu} = \frac{Ze g_N}{2M_p c} \vec{I}$$

$$\vec{A}(\vec{r}) = \frac{1}{4\pi} (\vec{\mu} \times \vec{r}) \frac{1}{r^3} \quad \text{magnetik alan}$$

$$\vec{B} = \vec{r} \times \vec{A} = -\frac{\vec{\mu}}{4\pi} \frac{r^2}{r^3} + \frac{1}{4\pi} \vec{r} (\vec{\mu} \cdot \vec{r}) \frac{1}{r^3}$$

$$\Rightarrow B_i = -\mu_j \frac{1}{4\pi} \frac{r^2}{r^3} + \frac{1}{4\pi} \mu_j \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r}$$

$$= \mu_j \delta_{ij} \delta(\vec{r}) + \frac{1}{4\pi} \mu_j \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r}$$

$$H_{hf} = -\vec{\mu}_e \cdot \vec{B} = -M_e M_i \delta(r) + \frac{1}{4\pi} M_e M_i \partial_{x_i}^2 \frac{1}{r}$$

Basit bir boyutlu pertürbasyonun $\vec{\mu}_e \cdot \vec{B} / a_0^3$ şeklinde olacağını gösterir

$$\langle H_{hf} \rangle \approx \frac{Ze^2 g \mu}{m_e \mu_B c^2} \frac{1}{a_0} \left(\frac{Z \alpha m_e c}{\hbar} \right)^2 \approx g \mu (Z \alpha)^4 m_e c^2 \left(\frac{\mu_B}{m_e} \right)$$

~ 5 yarıçapı civarında

Hydrojen atomunun $l=0$ durumunun yarıçapı a_0 ile uyarılır.

$$\int d^3r |\phi_{n0}(r)|^2 \left(-M_e M_i \delta(r) + \frac{1}{4\pi} M_e M_i \partial_{x_i}^2 \frac{1}{r} \right)$$

$|\phi_{n0}(r)|^2$ bir küresel simetrik fonksiyondur,

$$\int d^3r |\phi_{n0}(r)|^2 \partial_{x_i}^2 \frac{1}{r} = \frac{1}{3} \delta_{ij} \int d^3r |\phi_{n0}|^2 \partial_{x_i}^2 \frac{1}{r}$$

$\sim g \mu \delta(r)$

$$= -\frac{4\pi}{3}$$

$$= -\frac{4\pi}{3} \delta_{ij} \int d^3r |\phi_{n0}(r)|^2 \delta(r) \quad \dots -1 = -\frac{1}{3}$$

$$= -\frac{4\pi}{3} |\phi_{n0}(0)|^2$$

$$= -\frac{4}{3} M_e M_i |\phi_{n0}(0)|^2$$

$$\langle \phi_{n0} | H_{hf} | \phi_{n0} \rangle = -\frac{4}{3} \underbrace{\vec{M}_e \cdot \vec{M}}_{\frac{4}{n^3} \left(\frac{2\alpha m_e c}{\hbar} \right)^2} |\phi_{n0}(0)|^2$$

$$\langle H \rangle = \frac{4}{3} g_N \frac{m_e}{m_N} (2\alpha)^2 m_e c^2 \frac{1}{n^3} \frac{\vec{S} \cdot \vec{I}}{\hbar}$$

$$\vec{F} = \vec{S} + \vec{I}$$

$$\frac{\vec{S} \cdot \vec{I}}{\hbar} = \frac{\vec{F}^2 - \vec{S}^2 - \vec{I}^2}{2\hbar^2} = \frac{F(F+1) - 3/4 - I(I+1)}{2}$$

$$= \frac{1}{2} \begin{cases} I \\ -I-1 \end{cases} \quad \begin{array}{l} F = I + 1/2 \\ F = I - 1/2 \end{array}$$

$$\text{Hyd: } g_N \approx g_p \approx 5.56$$

○

Prob. 17.1

$$H_{SO} = \frac{1}{2m^2 c^2} \vec{S} \cdot \vec{L} \quad \frac{1}{r} \frac{dV(r)}{dr}$$

harmonischer Oszillator's Spektrum übereinstimmt?

$$H = -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} k r^2 \quad \hbar = m \omega^2$$

$$= -\frac{\hbar^2}{2m} \left\{ \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] \right\} + \frac{1}{2} k r^2$$

$$H\psi = E\psi \quad \psi = R(r) Y(\theta, \varphi)$$

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{Mk}{\hbar^2} r^2 + \frac{2M}{\hbar^2} E r^2$$

$$= -\frac{1}{Y} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \varphi^2} \right] = l(l+1)$$

$$Y = \Theta \Phi$$

$$\frac{1}{\Theta} \sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + l(l+1) \sin^2 \theta$$

$$= -\frac{1}{\Phi} \frac{d^2 \Phi}{d\varphi^2} = m^2$$

$$Y \equiv Y_{\ell}^m(\theta, \varphi) = (-1)^m \sqrt{\frac{2\ell+1}{4\pi}} \sqrt{\frac{(\ell-m)!}{(\ell+m)!}} P_{\ell}^m(\cos \theta) e^{im\varphi}$$

(2)

$$r = \sqrt{\hbar/m\omega} \rho$$

$$2E/\hbar\omega = \lambda$$

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{dR}{d\rho} \right) + \left(\lambda - \rho^2 - \frac{\ell(\ell+1)}{\rho^2} \right) R = 0$$

$$R = e^{-\rho^2/2} \Phi(\rho)$$

$$\frac{d^2 \Phi}{d\rho^2} + 2 \left(\frac{1}{\rho} - \rho \right) \frac{d\Phi}{d\rho} + \left(-3 + \lambda - \frac{\ell(\ell+1)}{\rho^2} \right) \Phi = 0$$

$$\Phi(\rho) = \sum_{k=0}^{\infty} a_k \rho^{k+s}$$

$$s = \begin{cases} \ell \\ -(\ell + 1) \end{cases}$$

$\rho = 0$ da Φ sınırlı $-(\ell+1)$ çözüm olmaz

$$\lambda - 3 = 2n \Rightarrow \lambda = 2n + 3 = \frac{2E}{\hbar\omega}$$

$$E_n = \left(n + \frac{3}{2} \right) \hbar\omega$$

$$\Phi(\rho) = \rho^{\ell} F(\rho) \quad z = \rho^2$$

$$z \frac{d^2 F}{dz^2} + \left(\ell + \frac{3}{2} - z \right) \frac{dF}{dz} + \left(\frac{n-\ell}{2} \right) F = 0$$

$$F = L_{\ell+\frac{1}{2}}^{n-\ell} (z) = L_{\frac{n-\ell}{2}}^{\ell+\frac{1}{2}} (\rho^2)$$

$$R(r) = N_{nl} e^{-m\omega r^2/2\hbar} \left[\sqrt{\frac{m\omega}{\hbar}} r \right]^l \left[\frac{l+1}{l} \left(\frac{m\omega}{\hbar} r^2 \right) \right]$$

$$= \sqrt{2} \left(\frac{m\omega}{\hbar} \right)^{3/4} \left[r \left(l + \frac{2}{3} \right) \left(\frac{l+l+1}{2} \right) \right]^{1/2}$$

$$\frac{dV(r)}{dr} = kr$$

○

$$H_{SO} = \frac{k}{2m^2c^2} \vec{S} \cdot \vec{L}$$

$$\vec{S} \cdot \vec{L} = \frac{1}{2} (\vec{J}^2 - \vec{L}^2 - \vec{S}^2)$$

$$\vec{S} \cdot \vec{L} \psi_{j=l+1/2, m_j=m+1/2} = \frac{\hbar^2}{2} l \psi_{j=l+1/2, m_j=m+1/2}$$

○

$$\vec{S} \cdot \vec{L} \psi_{j=l-1/2, m_j=m-1/2} = -\frac{\hbar^2}{2} (l+1) \psi_{j=l-1/2, m_j=m-1/2}$$

$$\langle H_{SO} \rangle = \frac{k}{2m^2c^2} \frac{\hbar^2}{2} \begin{cases} l \\ -(l+1) \end{cases}$$

4.

Extr: hätten wir polaren ablesen können

$$\vec{F} = \vec{r}, -\vec{r}$$

$$\vec{S}_1 = \frac{1}{2} \vec{\sigma}_1, \quad \vec{S}_2 = \frac{1}{2} \vec{\sigma}_2$$

elisch überg

$$V(\vec{r}) = V_1(r) + V_2(r) \left(3 \frac{(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) + V_3 \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

$$\vec{S} = \vec{S}_1 + \vec{S}_2$$

$$\vec{S} = \frac{1}{2} \left[3 \frac{(\vec{S} \cdot \vec{r})^2}{r^2} - \vec{S}^2 \right]$$

apfel-apfel.

$$\Rightarrow (\vec{S} \cdot \vec{r})^2 = \frac{1}{4} (\vec{\sigma}_1 \cdot \vec{r} + \vec{\sigma}_2 \cdot \vec{r})^2$$

$$= \frac{1}{4} [(\vec{\sigma}_1 \cdot \vec{r})^2 + (\vec{\sigma}_2 \cdot \vec{r})^2 + 2(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})]$$

$$(\vec{\sigma}_1 \cdot \vec{r})^2 = [x\sigma_{1x} + y\sigma_{1y} + z\sigma_{1z}]^2$$

$$= x^2 + y^2 + z^2 = r^2$$

$$(\vec{S} \cdot \vec{r})^2 = \frac{1}{4} (r^2 + (\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r}))$$

$$(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r}) = \frac{2}{1} (\vec{S} \cdot \vec{r})^2 - r^2$$

$$\frac{(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{4} = \frac{2}{1} \frac{(\vec{S} \cdot \vec{r})^2}{4} - r^2$$

$$\vec{S}^2 = \frac{\hbar^2}{4} (\vec{\sigma}_1^2 + \vec{\sigma}_2^2 + 2\vec{\sigma}_1 \cdot \vec{\sigma}_2) = \frac{\hbar^2}{4} (6I + 2\vec{\sigma}_1 \cdot \vec{\sigma}_2)$$

$$= \frac{\hbar^2}{2} (3I + \vec{\sigma}_1 \cdot \vec{\sigma}_2)$$

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 = \frac{2}{\hbar^2} \vec{S}^2 - 3I$$

$$\frac{3(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} = \frac{6}{\hbar^2} \frac{(\vec{S} \cdot \vec{r})^2}{r^2} - 3I$$

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 = \frac{2}{\hbar^2} \vec{S}^2 - 3I$$

$$\therefore = \frac{6}{\hbar^2} \frac{(\vec{S} \cdot \vec{r})^2}{r^2} - \frac{2}{\hbar^2} \vec{S}^2 = \frac{2}{\hbar^2} \left[3 \frac{(\vec{S} \cdot \vec{r})^2}{r^2} - \vec{S}^2 \right]$$

