449 Final

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In[2]:=
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Import["/Users/megantabbutt/Desktop/Quantum/Defs/448defs.m"]
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Notes about Citation Notation:

T.11 = Townsend Ch 11
All equation numbers not noted as a specific text are townsend: (11.24) = townsend equation 11.24 vs (Griffiths 11.24)

2) A Rb atom in the 50s state is in an electric field $\mathcal{E}$. In zero field the 50 p state has slightly higher energy than the 50 s, and the 49 p has slightly lower energy by very nearly the same amount, Δ. The radial integral ( ). Find the change in the 50 s energy as a function of electric field, for small fields.

Nondegenerate perturbation theory (Townsend Ch 11)

"First order energy shift" - (A section in T.11)

$$E_n{}^{(1)} = \left\langle \phi_n{}^{(0)} \middle| H_1 \middle| \phi_n{}^{(0)} \right\rangle \qquad (11.15)$$

Electric field E --> $H_1 = e\,Z\,\mathcal{E}$ (class notes and midterm 2)

$$E_{50\,s}{}^{(1)} = \left\langle \phi_{50\,s}{}^{(0)} \middle| H_1 \middle| \phi_{50\,s}{}^{(0)} \right\rangle = E_{50\,s}{}^{(1)} = \left\langle \phi_{50\,s}{}^{(0)} \middle| e\,Z\,\mathcal{E} \middle| \phi_{50\,s}{}^{(0)} \right\rangle$$

But the s state is spherically symmetric and the Z operator can be expressed in terms of Ylm's that will have a theta dependance so this is zero, as well z is odd but the matrix elements are the same so it will evaluate to zero.

"second order energy shift" - (A section in T.11)

$$E_n{}^{(2)} = \left\langle \phi_n{}^{(0)} \middle| H \middle| \phi_n{}^{(1)} \right\rangle \qquad (11.25)$$

$$E_n{}^{(2)} = \langle \phi_n{}^{(0)} | H | \phi_n{}^{(1)} \rangle = \text{SUM}[\frac{|\langle \phi_k{}^{(0)} | H | \phi_n{}^{(0)} \rangle|^2}{E_n{}^{(0)} - E_k{}^{(0)}}] \text{ for } k =! n \qquad (11.25)$$

Plug the 50s, 50p, 49p for n and k

$$E_{50\,s}{}^{(2)} = \frac{|\langle \phi_{50\,p}{}^{(0)} | H | \phi_{50\,s}{}^{(0)} \rangle|^2}{E_{50\,s}{}^{(0)} - E_{50\,p}{}^{(0)}} + \frac{|\langle \phi_{49\,p}{}^{(0)} | H | \phi_{50\,s}{}^{(0)} \rangle|^2}{E_{50\,s}{}^{(0)} - E_{49\,p}{}^{(0)}}, H = e Z \mathcal{E} \text{ (as previously stated)}$$

$$z = Y_{10}\, 2\, r\, \text{Sqrt}[\pi / 3] \qquad \text{(Wikipedia: Table of spherical harmonics)}$$

$$E_{50\,s}{}^{(2)} = \frac{|\langle \phi_{50\,p}{}^{(0)} | H | \phi_{50\,s}{}^{(0)} \rangle|^2}{E_{50\,s}{}^{(0)} - E_{50\,p}{}^{(0)}} + \frac{|\langle \phi_{49\,p}{}^{(0)} | H | \phi_{50\,s}{}^{(0)} \rangle|^2}{E_{50\,s}{}^{(0)} - E_{49\,p}{}^{(0)}}$$

$$E_{50\,s}{}^{(2)} = \frac{|\langle \phi_{50\,p}{}^{(0)} | e Y_{10}\, 2\, r\, \text{Sqrt}[\pi/3]\, \mathcal{E} | \phi_{50\,s}{}^{(0)} \rangle|^2}{-\Delta} + \frac{|\langle \phi_{49\,p}{}^{(0)} | e Y_{10}\, 2\, r\, \text{Sqrt}[\pi/3]\, \mathcal{E} | \phi_{50\,s}{}^{(0)} \rangle|^2}{\Delta}$$

$$E_{50\,s}{}^{(2)} = 2\, e\, \mathcal{E}\, \text{Sqrt}\left[\frac{\pi}{3}\right] \left(\frac{|\langle \phi_{50\,p}{}^{(0)} | Y_{10}\, r | \phi_{50\,s}{}^{(0)} \rangle|^2}{-\Delta} + \frac{|\langle \phi_{49\,p}{}^{(0)} | Y_{10}\, r | \phi_{50\,s}{}^{(0)} \rangle|^2}{\Delta} \right)$$

$$E_{50\,s}{}^{(2)} = \frac{2\, e\, \mathcal{E}\, \text{Sqrt}\left[\frac{\pi}{3}\right]}{\Delta} \left(|\langle \phi_{49\,p}{}^{(0)} | Y_{10}\, r | \phi_{50\,s}{}^{(0)} \rangle|^2 - |\langle \phi_{50\,p}{}^{(0)} | Y_{10}\, r | \phi_{50\,s}{}^{(0)} \rangle|^2 \right)$$

$$\int d r P_{50\,s}(r)\, r P_{np}(r) = n^2 a \qquad \text{(use Griffiths notation, a = a0)}$$

$$E_{50\,s}{}^{(2)} = \frac{4\, e\, \mathcal{E}\, \frac{\pi}{3}}{\Delta} \left(|\langle \phi_{49\,p}{}^{(0)} | Y_{10}\, r | \phi_{50\,s}{}^{(0)} \rangle|^2 - |\langle \phi_{50\,p}{}^{(0)} | Y_{10}\, r | \phi_{50\,s}{}^{(0)} \rangle|^2 \right)$$

$$E_{50\,s}{}^{(2)} = \frac{4\, e\, \mathcal{E}\, \frac{\pi}{3}}{\Delta} \left(\frac{5\,764\,801\, a^2}{4\,\pi} - \frac{1\,562\,500\, a^2}{\pi} \right)$$

$$E_{50\,s}{}^{(2)} = -\frac{161\,733.\, a^2\, e\, \mathcal{E}}{\Delta}$$

In[10]:=

```
(Integrate[(49^2 * a) SphericalHarmonicY[1, -1, θ, ϕ] *
    SphericalHarmonicY[1, 0, θ, ϕ] * SphericalHarmonicY[0, 0, θ, ϕ] * Sin[θ],
   {θ, 0, π}, {ϕ, 0, 2 π}] + Integrate[(49^2 * a) SphericalHarmonicY[1, 0, θ, ϕ] *
    SphericalHarmonicY[1, 0, θ, ϕ] * SphericalHarmonicY[0, 0, θ, ϕ] *
    Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}] + Integrate[
   (49^2 * a) SphericalHarmonicY[1, 1, θ, ϕ] * SphericalHarmonicY[1, 0, θ, ϕ] *
    SphericalHarmonicY[0, 0, θ, ϕ] * Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}])^2
```

Out[10]=

$$\frac{5\,764\,801\, a^2}{4\,\pi}$$

In[11]:=

```
(Integrate[(50^2 * a) SphericalHarmonicY[1, -1, θ, ϕ] *
    SphericalHarmonicY[1, 0, θ, ϕ] * SphericalHarmonicY[0, 0, θ, ϕ] * Sin[θ],
   {θ, 0, π}, {ϕ, 0, 2 π}] + Integrate[(50^2 * a) SphericalHarmonicY[1, 0, θ, ϕ] *
    SphericalHarmonicY[1, 0, θ, ϕ] * SphericalHarmonicY[0, 0, θ, ϕ] *
    Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}] + Integrate[
   (50^2 * a) SphericalHarmonicY[1, 1, θ, ϕ] * SphericalHarmonicY[1, 0, θ, ϕ] *
    SphericalHarmonicY[0, 0, θ, ϕ] * Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}])^2
```

Out[11]=

$$\frac{1\,562\,500\, a^2}{\pi}$$

In[12]:=

$$\frac{5\,764\,801\, a^2}{4\,\pi} - \frac{1\,562\,500\, a^2}{\pi}$$

Out[12]=

$$-\frac{485\,199\, a^2}{4\,\pi}$$

In[19]:=

$$-\frac{485\,199\, a^2}{4\,\pi} * \frac{4\, e\, \mathcal{E}\, \frac{\pi}{3}}{\Delta} \; // \; N$$

Out[19]=

$$-\frac{161\,733.\, a^2\, e\, \mathcal{E}}{\triangle}$$