Physik IV - Lösungen - Serie 10

18. Mai 2011

1)
$$\left\langle \frac{1}{r} \right\rangle = \int \psi^*(r,\theta,\varphi)\, \frac{1}{r}\, \psi(r,\theta,\varphi)\, d^3r =$$

$$= \int_0^\infty |R_{nl}(r)|^2 \frac{1}{r} \cdot r^2\, dr \underbrace{\int Y_{lm}^*(\theta,\varphi)\, Y_{lm}(\theta,\varphi)\, \sin\theta\, d\theta\, d\varphi}_{1 \text{ due to normalization}}$$

1s: with $R_{10}(r) = 2\, a_0^{-\frac{3}{2}}\, e^{-r/a_0}$

$$= \frac{4}{a_0^3} \int_0^\infty r\, e^{-2r/a_0}\, dr =$$

with $\int_0^\infty r^n e^{-ar}\, dr = \frac{n!}{a^{n+1}}$

$$= \frac{4}{a_0^3} \cdot \frac{a_0^2}{4} = \frac{1}{a_0} \quad \Rightarrow \quad E_1 = -\frac{e^2}{4\pi\varepsilon_0} \cdot \frac{1}{2a_0}$$

2p with $R_{21} = \frac{2}{\sqrt{3}} \left(\frac{1}{2a_0}\right)^{\frac{3}{2}} \left(\frac{r}{2a_0}\right) e^{-r/2a_0}$

$$\left\langle \frac{1}{r} \right\rangle_{21} = \int_0^\infty r \cdot R_{21}^2\, dr = \frac{4}{3}\, \frac{1}{8a_0^3}\, \frac{1}{4a_0^2} \int r^3 e^{-r/a_0}\, dr =$$

$$= \frac{1}{3 \cdot 8 a_0^5} \cdot 3 \cdot 2 \cdot a_0^4 = \frac{1}{4a_0} \quad \Rightarrow \quad E_2 = -\frac{e^2}{4\pi\varepsilon_0} \cdot \frac{1}{2} \cdot \frac{1}{4a_0}$$

$$\Rightarrow \Delta E = E_2 - E_1 = \frac{e^2}{4\pi\varepsilon_0}\, \frac{1}{2a_0}\left(1 - \frac{1}{4}\right) = 1.64 \times 10^{-18}\, J \mathrel{\hat{=}} 10\, eV$$

$$\omega = \frac{\Delta E}{\hbar} = 15.5 \times 10^{15}\, rad/s \mathrel{\hat{=}} 2.46 \times 10^{15}\, Hz \mathrel{\hat{=}} \lambda = 121.7\, nm$$

2 (a) Probability to find electron @ $r > a_0$ is

$$P(r>a_0) = \int_{a_0}^{\infty} |R|^2 r^2 \, dr$$

$$= \int_{a_0}^{\infty} \frac{4}{a_0^3} r^2 e^{-2r/a_0} \, dr$$

$$= \frac{4}{a_0^3} \frac{\partial^2}{\partial\beta^2} \int_{a_0}^{\infty} e^{-\beta r} \, dr$$

$$= \frac{4}{a_0^3} \left[\frac{\partial^2}{\partial\beta^2} \left(\frac{-1}{\beta} e^{-\beta r} \right) \right]_{a_0}^{\infty}$$

$$= \frac{4}{a_0^3} \left[-e^{-\beta r} \left(\frac{2r}{\beta^2} + \frac{r^2}{\beta} + \frac{2}{\beta^3} \right) \right]_{a_0}^{\infty} = \frac{5}{e^2} = \underline{\underline{0.68}}$$

INTEGRATION TRICK

$$\int r^n e^{-\beta r} \, dr = \left(-\partial/\partial\beta\right)^n \int e^{-\beta r} \, dr = \left(-\partial/\partial\beta\right)^n \left(-e^{-\beta r}/\beta\right)$$

Use $\beta \equiv 2/a_0$

$$\langle r \rangle = \int_0^{\infty} |R|^2 r . r^2 \, dr = \int_0^{\infty} \frac{4}{a_0^3} r^3 e^{-\beta r} \, dr$$

$$= \frac{4}{a_0^3} \frac{-\partial^3}{\partial\beta^3} \int_0^{\infty} e^{-\beta r} \, dr$$

$$= \frac{4}{a_0^3} \left[-e^{-\beta r} \left(\frac{6}{\beta^4} + \frac{6r}{\beta^3} + \frac{3r^2}{\beta^2} + \frac{r^3}{\beta} \right) \right]_0^{\infty}$$

$$= \frac{4}{a_0^3} \cdot 6 \cdot \left(\frac{a_0}{2}\right)^4 = \frac{3}{2} a_0 \quad ///$$

Max. of probability distribution is at

$$\frac{\partial}{\partial r}\left(|R|^2 r^2\right) = 0 \Rightarrow$$

$$\frac{\partial}{\partial r}\left(r^2 e^{-2r/a_0}\right) = 0 \Rightarrow$$

$$-\frac{2}{a_0} r^2 e^{-2r/a_0} + 2r e^{-2r/a_0} = 0$$

$$\Rightarrow r = a_0$$

Most likely value of r is $r = a_0$.

Average value of r is $r = \frac{3}{2} a_0$.

(3) Transitions & Zeeman Effect

(a) $\Delta l = \pm 1 \quad \Delta m_l = 0, \pm 1.$

$n=1$: 1s orbital $l=0$, $m_l = 0$

$n=2$: 2s, $l=0$, $m_l=0$

2p, $l=1$, $m_l = -1, 0, +1$.

possible transitions

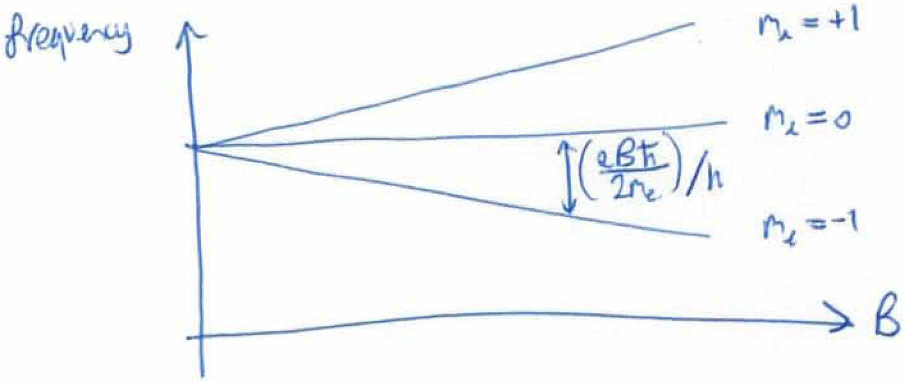
3 possible transitions 1s → 2p, $m_l = -1$

→ 2p, $m_l = 0$

→ 2p, $m_l = +1$

(b) They are of the same energy @ $B=0$ $\left[\Delta E = R_\infty\left(\frac{1}{n^2} - \frac{1}{m^2}\right) = \frac{3}{4}R_\infty\right]$

As $B\uparrow$, the Zeeman effect must be included $\Delta E_z = 0, \pm \frac{eB}{2m_e}(\hbar)$



(c) $\Delta f = \frac{eB\hbar}{2m_e}/h = \begin{cases} 1.4 \times 10^{11} \text{ Hz} = 140 \text{ GHz} \quad (B = 10\text{T}) \\ 1.4 \times 10^{6} \text{ Hz} = 1.4 \text{ MHz} \quad (B = 10^{-4}\text{T}) \end{cases}$

4. **Stern-Gerlach experiment**
At this temperature, all the H-atoms in the oven are in their ground state and hence the internal degrees of freedom are frozen out and do not contribute to the temperature of the system. Let the SG-magnet be oriented in the x-direction. From the equipartition theorem for the CM degree of freedom, we have $\langle K \rangle = \frac{1}{2}m\langle v_x^2 \rangle = kT/2$, hence $\langle v_x^2 \rangle = \sqrt{kT/m}$. This is a very rough argument as the atoms emanating from the hole are not the 'typical' members of the ensemble (it turns out that for atoms leaving the hole, $\langle v_x^2 \rangle \approx 4kT/m$). Once out, the force that each atom experiences due to the inhomogeneous field is given by

$$F_z = -\frac{\partial B_z}{\partial z}\mu_B g_s m_s = \pm\mu_B \frac{\partial B_z}{\partial z} \tag{1}$$

The average time of flight is given by $t = L/\sqrt{\langle v_x^2 \rangle}$. The center-to-center distance of the two spots on the detector will then be given by

$$\Delta z = (F_z/m)t^2 = \mu_B L^2(\partial B_z/\partial z)/kT \approx 1.6\,\mathrm{cm}. \tag{2}$$

5) $\vec{\mu}_s = -\frac{e}{m}\hat{\vec{S}}$

$$H = -\vec{\mu}_s \cdot \vec{B} = +\frac{e}{m}\hat{\vec{S}}\cdot\vec{B} = \frac{e}{m}\begin{pmatrix}\hat{S}_x\\ \hat{S}_y\\ \hat{S}_z\end{pmatrix}\cdot\begin{pmatrix}0\\0\\B_z\end{pmatrix} =$$

$$= \frac{eB_z}{m}\hat{S}_z$$

state $|m_s\rangle$ of the electron either $|-\frac{1}{2}\rangle$ or $|+\frac{1}{2}\rangle$

the quantum numbers n, l, m_l don't play a role here.

potential energy

$$\hat{S}_z\,|\pm\tfrac{1}{2}\rangle = \pm m_s\hbar\,|\pm\tfrac{1}{2}\rangle$$

$$U_{pot} = \langle m_s|H|m_s\rangle =$$

$$= \langle\pm\tfrac{1}{2}|\ \frac{eB_z}{m}\hat{S}_z\,|\pm\tfrac{1}{2}\rangle$$

$$= \pm\frac{e\hbar}{2m}B_z = \pm\mu_B \qquad \Delta U = 2\mu_B B_z$$

For example, if |Bz|= 1T: $\Delta U = 2\times 9.274\ 10^{-24}\,J \mathrel{\hat{=}} 58\,\mu eV$

b) $H\,|m_s(t)\rangle = i\hbar\frac{d}{dt}|m_s(t)\rangle$

$$-\frac{i}{\hbar}\underbrace{\frac{2\mu_B B_z}{\hbar}}_{\alpha}\hat{S}_z\,|m_s(t)\rangle = \frac{d}{dt}|m_s(t)\rangle$$

$|\frac{1}{2}(t)\rangle$: $\quad -i\frac{\alpha}{2}\,|\frac{1}{2}(t)\rangle = \frac{d}{dt}|\frac{1}{2}(t)\rangle \qquad$ with $\hat{S}_z|\frac{1}{2}\rangle = \frac{\hbar}{2}|\frac{1}{2}\rangle$

$$\Rightarrow |\tfrac{1}{2}(t)\rangle = e^{-i\frac{\alpha}{2}t}\,|\tfrac{1}{2}(0)\rangle$$

$|-\frac{1}{2}(t)\rangle$: $\quad |-\frac{1}{2}(t)\rangle = e^{i\frac{\alpha}{2}t}\,|-\frac{1}{2}(0)\rangle$

Time evolution gives an additional phase factor.

$$\frac{\alpha}{2} = \frac{\mu_B B}{\hbar}$$

c) $|m_s(0)\rangle = \frac{1}{\sqrt{2}}\left[|\tfrac{1}{2}(0)\rangle + |-\tfrac{1}{2}(0)\rangle\right]$

$$|m_s(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{-i\frac{\alpha}{2}t}|\tfrac{1}{2}(0)\rangle + e^{i\frac{\alpha}{2}t}|-\tfrac{1}{2}(0)\rangle\right]$$

$$\langle m_s(t)|\hat{S}_x|m_s(t)\rangle = \frac{1}{2}\langle m_s(t)|\hat{S}_+ + \hat{S}_-|m_s(t)\rangle$$

$$= \frac{1}{4}\left[e^{+i\frac{\alpha}{2}t}\langle\tfrac{1}{2}| + e^{-i\frac{\alpha}{2}t}\langle-\tfrac{1}{2}|\right]\left(\hat{S}_+ + \hat{S}_-\right)\left[e^{-i\frac{\alpha}{2}t}|\tfrac{1}{2}\rangle + e^{i\frac{\alpha}{2}t}|-\tfrac{1}{2}\rangle\right]$$

$$S_+|\tfrac{1}{2}\rangle = 0 \; ; \; S_-|\tfrac{1}{2}\rangle = \hbar|-\tfrac{1}{2}\rangle$$

$$S_+|-\tfrac{1}{2}\rangle = \hbar|+\tfrac{1}{2}\rangle \; ; \; S_-|-\tfrac{1}{2}\rangle = 0$$

$$\langle\pm\tfrac{1}{2}|\mp\tfrac{1}{2}\rangle = 0$$

$$= \frac{\hbar}{4}\left[e^{i\alpha t} + e^{-i\alpha t}\right] = \frac{\hbar}{2}\cos\alpha t = \langle S_x\rangle$$

α ... Larmor frequency $= \frac{2\mu_B B}{\hbar}$

Such spin oscillations are used for nuclear magnetic resonance techniques (with the nuclear spin) also for medical use (Magnetic resonance imaging).

Mathematica Aufgabe 7 - Bahndrehimpulseigenfunktion

Load Packages :

In[6]:=
```
<< PhysicalConstants`
<< VectorAnalysis`
(*for solving the differential equations in spherical coordinates*)
SetOptions[Plot, BaseStyle → {FontSize → 14, FontFamily -> "Arial"},
  PlotStyle → {AbsoluteThickness[2]}];
SetCoordinates[Spherical[r, θ, ϕ]];
```

Bestimmung des Drehimpulses und Zerlegung in Kugelflächenfunktionen :

Bahndrehimpulsoperator : $\Lambda^2 = -\hbar^2 \left(\frac{1}{\sin[\theta]^2} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin[\theta]} \frac{\partial}{\partial \theta} \sin[\theta] \frac{\partial}{\partial \theta} \right)$

In[30]:=
$$\text{Λ2}[\psi\_, \theta\_, \phi\_] := -\hbar^2 \left(\frac{1}{\text{Sin}[\theta]^2} \text{D}[\psi, \{\phi, 2\}] + \frac{1}{\text{Sin}[\theta]} \text{D}[\text{Sin}[\theta]\ \text{D}[\psi, \theta], \theta] \right)$$

In[31]:=
```
ψ = (x + y + 3 z) f[r] /. {x → r Sin[θ] Cos[ϕ], y → r Sin[θ] Sin[ϕ], z → r Cos[θ]}
```

Out[31]=
$$\frac{e^{-r/2} \left(3\, r \,\text{Cos}[\theta] + r \,\text{Cos}[\phi]\, \text{Sin}[\theta] + r \,\text{Sin}[\theta]\, \text{Sin}[\phi]\right)}{2 \sqrt{6}}$$

In[32]:=
$$\text{Solve}\left[\text{Λ2}[\psi, \theta, \phi] == \lambda \hbar^2 \psi, \lambda\right] \text{ // FullSimplify}$$

Out[32]=
$\{\{\lambda \to 2\}\}$

aus $\lambda = l\,(l + 1)$ folgt somit $l = 1$.

Die Wellenfunktion kann somit als Superposition von Kugelflächenfunktionen geschrieben werden, wobei wir zur Bestimmung der Koeffizienten die Orthonormalitätsrelationen ($\int Y^*_{lm}\, Y_{l'\,m'}\, d\Omega = \delta_{l\,l'}\, \delta_{m\,m'}$) ausnutzen.

In[33]:=
```
coeffm1 =
 Integrate[ψ SphericalHarmonicY[1, -1, θ, ϕ]* Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}] / (r f[r])
coeff0 = Integrate[ψ SphericalHarmonicY[1, 0, θ, ϕ]* Sin[θ],
   {θ, 0, π}, {ϕ, 0, 2 π}] / (r f[r])
coeffp1 = Integrate[ψ SphericalHarmonicY[1, 1, θ, ϕ]* Sin[θ],
   {θ, 0, π}, {ϕ, 0, 2 π}] / (r f[r])
```

Out[33]= $(1 + i)\sqrt{\frac{2\pi}{3}}$

Out[34]= $2\sqrt{3\pi}$

Out[35]= $(-1 + i)\sqrt{\frac{2\pi}{3}}$

In[36]:=
```
Y[l_Integer, m_Integer, θ_, ϕ_] := SphericalHarmonicY[l, m, θ, ϕ]
```

Radialteil

In[37]:=
```
wavenumber = Solve[-1 + 1/(a k) - l == nr, k][[1]];
radial[r_, n_, l_] =
  Cr e^(-k r) r^l LaguerreL[-1 + 1/(a k) - l, 1 + 2 l, 2 k r] /. wavenumber //. {nr → n - l - 1};
Table[Table[
   CNorm[i, j, a_] = Cr /. Solve[Integrate[
         Evaluate[radial[r, i, j]^2] r^2, {r, 0, ∞}, Assumptions → {a > 0}] == 1, Cr][[2]],
   {j, 0, i - 1}],
  {i, 1, 6}];
Rnl[r_, n_, l_, a_: 1] := CNorm[n, l, a] e^(-r/(a n)) r^l LaguerreL[-1 + n - l, 1 + 2 l, 2 r/(a n)]
```

Minimales n für l = 1 : $n_{min} = 2$

In[41]:=
```
f[r_, a_: 1] := Rnl[r, 2, 1, a] / r
f[r]
```

Out[42]= $\frac{e^{-r/2}}{2\sqrt{6}}$

Wellenfunktion :

In[43]:=
```
ψcomplete[r_, θ_, ϕ_, a_: 1] :=
 f[r, a] r (coeffm1 Y[1, -1, θ, ϕ] + coeff0 Y[1, 0, θ, ϕ] + coeffp1 Y[1, 1, θ, ϕ])
```

In[44]:=
```
coordinateline = Graphics3D[{Thick, Line[{{-300, 0, 0}, {300, 0, 0}}],
     Line[{{0, -300, 0}, {0, 300, 0}}], Line[{{0, 0, -300}, {0, 0, 300}}]}];
myplotrange = {-0.2, 0.2};
```

SphericalPlot

In[46]:=
```
SphericalPlot3D[Evaluate[ψcomplete[1, θ, ϕ]* ψcomplete[1, θ, ϕ]], {θ, 0, π}, {ϕ, 0, 2 π},
   PlotRange → myplotrange, PlotStyle → Directive[Orange, Specularity[White, 10]],
   Boxed → False, Axes → False, PlotPoints → 4];
Show[%, coordinateline]
```

Out[47]=