1992

ϕ507 Problems Assigned: 1/17. Due: 1/27/92. HW1 (1) file

(1) [15 pts]. The ODE: $zf'' + (b-z)f' - af = 0$, a & b = cnsts, for $f = f(z)$, is the confluent hypergeometric equation. (A) By direct substitution, show that a series solution is: $f(z) = F(a;b;z) = \sum_{k=0}^{\infty} [(a)_k/(b)_k] \frac{z^k}{k!}$, w/ $(a)_k = a(a+1)\cdots(a+k-1)$ & $(a)_0 = 1$, the Pochhammer symbol. (B) Let $|z| \to$ large, and note $(a)_k = \Gamma(k+a)/\Gamma(a)$. By examining the dominant terms in the series for F, and using suitable approximations for the Γ-fcns, show that for k "large", the k^{th} term in the series is $\sim [\Gamma(b)/\Gamma(a)]\, z^k/(k-(a-b))!$ Use this to show that for large (+)ve z (z real): $F(a;b;z) \sim [\Gamma(b)/\Gamma(a)]\, z^{a-b} e^z$. (C) Use the result of part (B) to show that for large (−)ve z (again real): $F(a;b;z) \sim [\Gamma(b)/\Gamma(b-a)](-z)^{-a}$.

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(2) Verify that: $\mathrm{erf}(x) = (2/\sqrt{\pi})\, x\, F(\frac{1}{2}; \frac{3}{2}; -x^2)$, F = confluent hypergeometric fcn. Find an expression for $\mathrm{erf}(x)$, correct to $\mathcal{O}(x^3)$, as $x \to 0$.

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(3) A QM system consists of two particles, of masses m_1 & m_2. Express the operators for total momentum $\hat{\mathbf{P}} = \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2$ and total ∡ momentum $\hat{\mathbf{L}} = \hat{\mathbf{l}}_1 + \hat{\mathbf{l}}_2$ in terms of the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and center-of-mass coordinate $\mathbf{R} = (m_1\mathbf{r}_1 + m_2\mathbf{r}_2)/(m_1+m_2)$. Show that the kinetic energy part of the Hamiltonian, viz $\hat{K} = \frac{1}{2m_1}\hat{\mathbf{p}}_1^2 + \frac{1}{2m_2}\hat{\mathbf{p}}_2^2$ can be put in the form: $\hat{K} = -(\hbar^2/2M)\nabla_R^2 - (\hbar^2/2\mu)\nabla_r^2$, w/ $M = m_1+m_2$ & $\mu = m_1m_2/(m_1+m_2)$.

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(4) [15 pts]. Consider a central potential of form: $V(r) = -\frac{B}{r} + \frac{A}{r^2}$; B & A are (+)ve cnsts.
(A) Sketch $V(r)$ vs. r. What physical system might be represented by such a potential?
(B) Write the radial eqtn in dimensionless variables ("atomic units" here are: length $a_0 = \frac{\hbar^2}{mB}$, energy $E_0 = \frac{B}{a_0}$). Find the radial wavefcn $R(\rho)$, and show that the bound state energies are: $\boxed{E_{n\ell} = -\frac{1}{2}E_0/(n+\Delta_\ell)^2}$, $n = 1,2,3,\ldots$ and $\ell = 0,1,\ldots,(n-1)$, just as for H-atoms. The "quantum defect" Δ_ℓ lifts the ℓ-degeneracy. Find an exact expression for Δ_ℓ.
(C) Now approximate $E_{n\ell}$ through terms of $\mathcal{O}(A)$. In a given state n, how are the ℓ-states arranged? Sketch an energy-level diagram for $n=1,2,3$. What is the energy spread in level n?

ϕ507 Solutions

① [15 pts]. Confl. HyperGeom. Eqtn: series solution & asymptotics for $|z| \to \infty$.

(A) By directly differentiating the series for $F = F(a;b;z)$, we find

$$\rightarrow \frac{dF}{dz} = \sum_{k=1}^{\infty} \frac{(a)_k}{(b)_k} \cdot \frac{z^{k-1}}{(k-1)!} = \sum_{k=0}^{\infty} \frac{(a)_{k+1}}{(b)_{k+1}} \cdot \frac{z^k}{k!}. \qquad (1)$$

But: $(a)_{k+1} = a(a+1)_k$, trivially. In fact: $\underline{(a)_{k+n} = \overbrace{a(a+1)\cdots(a+n-1)}^{(a)_n}(a+n)_k}$. So...

$$\frac{dF}{dz} = \frac{a}{b}\sum_{k=0}^{\infty} \frac{(a+1)_k}{(b+1)_k} \cdot \frac{z^k}{k!} = \frac{a}{b} F(a+1; b+1; z);$$

and

$$\frac{d^2F}{dz^2} = \frac{a(a+1)}{b(b+1)} F(a+2; b+2; z). \qquad (2)$$

Plug these results into the ODE, viz: $zF'' + (b-z)F' - aF = 0$, to obtain...

$$\frac{a(a+1)}{b(b+1)} zF(a+2;b+2;z) + (b-z)\frac{a}{b}F(a+1;b+1;z) - aF(a;b;z) \overset{(?)}{=} 0,$$

i.e.

$$\rightarrow \sum_{k=0}^{\infty} \frac{z^{k+1}}{k!}\left[\frac{(a)_{k+2}}{(b)_{k+2}} - \frac{(a)_{k+1}}{(b)_{k+1}}\right] + a\sum_{k=0}^{\infty}\frac{z^k}{k!}\left[\frac{(a+1)_k}{(b+1)_k} - \frac{(a)_k}{(b)_k}\right] \overset{(?)}{=} 0. \qquad (3)$$

We have used the above rule $(a)_{k+n} = (a)_n (a+n)_k$. Now we must prove that Eq. (3) is an <u>identity</u>... i.e. remove the (?)... to show the proposition (that the series for F is actually a solution to the confluent hypergeom. eqtn). First, note that the $k=0$ term in the 2nd sum LHS in Eq. (3) is $\equiv 0$, so that sum can be written as: $a\sum_{k=0}^{\infty} \frac{z^k}{(k+1)!}\left[\frac{(a+1)_{k+1}}{(b+1)_{k+1}} - \frac{(a)_{k+1}}{(b)_{k+1}}\right]$. Combined with the 1st sum...

$$\rightarrow \sum_{k=0}^{\infty} \frac{z^{k+1}}{k!}\left\{\frac{(a)_{k+2}}{(b)_{k+2}}\left[1+\frac{b}{k+1}\right] - \frac{(a)_{k+1}}{(b)_{k+1}}\left[1+\frac{a}{k+1}\right]\right\} \overset{(?)}{=} 0. \qquad (4)$$

The identity is proven once we show the $\{\ \} \equiv 0$. In turn, the $\{\ \} \overset{(?)}{=} 0$ requires $(b+k+1)(a)_{k+2}/(b)_{k+2} \overset{(?)}{=} (a+k+1)(a)_{k+1}/(b)_{k+1}$. But this is clearly true, since: $(b+k+1)/(b)_{k+2} = 1/(b)_{k+1}$ & $(a+k+1)(a)_{k+1} = (a)_{k+2}$. Thus, in Eq. (4), the $\{\ \} \equiv 0$, <u>and we have shown that</u>: $\underline{F = \sum_{k=0}^{\infty}[(a)_k/(b)_k]\frac{z^k}{k!}}$ <u>satisfies</u> $\underline{zF'' + (b-z)F' - aF = 0}$. <u>QED.</u>

(B) With $(a)_k = \Gamma(k+a)/\Gamma(a)$, the series for $F(a;b;z)$ is...

$$\rightarrow F(a;b;z) = \frac{\Gamma(b)}{\Gamma(a)} \sum_{k=0}^{\infty} \zeta_k, \quad \zeta_k = \frac{\Gamma(k+a)}{\Gamma(k+b)} \cdot \frac{z^k}{k!}. \tag{5}$$

The series converges for all z, and for $|z| \to \infty$, the terms with large k dominate. For $k \to$ large, we use the identity: $\lim_{k\to\infty}\left\{k^{b-a}\left[\frac{\Gamma(k+a)}{\Gamma(k+b)}\right]\right\} = 1$,¶ to write approx'ly:

$$\rightarrow \frac{\Gamma(k+a)}{\Gamma(k+b)} \simeq k^{a-b} \simeq \frac{\Gamma(k)}{\Gamma(k-(a-b))} \simeq k!/(k-(a-b))!, \text{ for } k \to \text{large}. \tag{6}$$

$$\xrightarrow{\text{so}} \zeta_k \simeq z^k/(k-(a-b))! = (z^{a-b})\frac{z^K}{K!}, \text{ w/ } K = k-(a-b). \tag{7}$$

The first expression for ζ_k shows that $F \sim \sum_k^{\infty} [\Gamma(b)/\Gamma(a)]\, z^k/(k-(a-b))!$, as required, where the lower summation limit can be lifted from $k=0$ because the terms with large k dominate. If we use the second expression for ζ_k in Eq. (7) in the original series for F...

$$\boxed{F(a;b;z) \sim \frac{\Gamma(b)}{\Gamma(a)} z^{a-b} \sum_K^{\infty} \frac{z^K}{K!} \sim [\Gamma(b)/\Gamma(a)]\, z^{a-b} e^z}, \quad z \to +\infty. \tag{8}$$

In the sum here, again K is "large" ($K \simeq k \to$ large, when $k \gg |a-b|$), and the starting point in the sum is not crucial. We are of course excluding some powers of z in taking $\sum_K^{\infty} z^K/K! \sim e^z$ [they are listed in NBS # (13.5.1)]. That z is (+)ve in Eq. (8) can be inferred from its integral form.*

(C) When $z = -|z|$ is large and (−)ve, use the Kummer transform in Eq. (8), i.e. use $F(a;b;-|z|) = e^{-|z|} F(b-a;b;|z|)$. Then we have immediately...

$$\boxed{F(a;b;z) \sim [\Gamma(b)/\Gamma(b-a)](-z)^{-a}}, \quad z \to (-)\infty. \tag{9}$$

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* $F(a;b;z) = [\Gamma(b)/\Gamma(a)\Gamma(b-a)] \int_0^1 e^{zt} t^{a-1}(1-t)^{b-a-1} dt$. If $|z| \to \infty$, and z is (−)ve, evidently $F \to 0$ (as in Eq. (9)). Only way to match $F \to$ large, per Eq. (8), is to have z (+)ve.

¶ "NBS Handbook of Math Fcns", M. Abramowitz & I. A. Stegun, formula # (6.1.46).

ϕ 507 Solutions

② Verify that: $erf(x) = (2/\sqrt{\pi})\, x\, F(\frac{1}{2}; \frac{3}{2}; -x^2)$, F = confl. hypergeom. fcn.

1) An integral rep^n for $F(a;b;z)$ -- per class notes, or NBS Handbook # (13.2.1) -- is

$$F(a;b;z) = [\Gamma(b)/\Gamma(a)\Gamma(b-a)] \int_0^1 e^{zt}\, t^{a-1}(1-t)^{b-a-1}\, dt \quad \left\{ \begin{array}{l} \text{for all } z, \text{ when:} \\ \mathrm{Re}\, b > \mathrm{Re}\, a > 0; \end{array} \right.$$

$$\xrightarrow{\text{Sq}} F(\tfrac{1}{2}; \tfrac{3}{2}; -x^2) = [\Gamma(\tfrac{3}{2})/\Gamma(\tfrac{1}{2})\Gamma(1)] \int_0^1 e^{-tx^2} \frac{1}{\sqrt{t}} \cdot 1 \cdot dt. \qquad (1)$$

2) In Eq. (1), $\Gamma(1) = 0! = 1$, $\Gamma(\frac{1}{2}) = \sqrt{\pi}$ and $\Gamma(\frac{3}{2}) = \frac{1}{2}\sqrt{\pi}$ [NBS # (6.1.8 & 9)]. Put in these values, and change integration variables from t to u, where ...

$$u^2 = tx^2 \Rightarrow \sqrt{t} = \frac{u}{x}, \text{ and: } dt = \frac{2u\,du}{x^2}$$

$$\text{So } F(\tfrac{1}{2}; \tfrac{3}{2}; -x^2) = [\cancel{\tfrac{1}{2}}] \int_0^x e^{-u^2} \frac{x}{u} \cdot \frac{\cancel{2}u\,du}{x^2} = \frac{1}{x} \int_0^x e^{-u^2} du$$

$$\xrightarrow{\text{by}} \int_0^x e^{-u^2} du = x\, F(\tfrac{1}{2}; \tfrac{3}{2}; -x^2). \qquad (2)$$

3) The error fcn $erf(x)$ is, by defn [e.g. NBS # (7.1.1)] ...

$$\rightarrow erf(x) = (2/\sqrt{\pi}) \int_0^x e^{-u^2} du. \qquad (3)$$

Comparison with Eq. (2) shows immediately, as required ...

$$\boxed{erf(x) = (2/\sqrt{\pi})\, x\, F(\tfrac{1}{2}; \tfrac{3}{2}; -x^2).} \qquad (4)$$

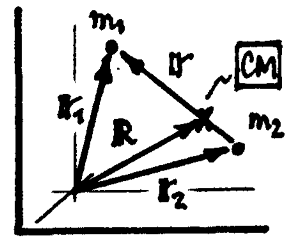
4) As $z \to 0$, $F(a;b;z) \simeq 1 + (a/b)z$. Use of this relation in Eq. (4) gives

$$\rightarrow \underline{\underline{erf(x) \simeq \frac{2}{\sqrt{\pi}}\, x\left(1 - \tfrac{1}{3}x^2 + \cdots\right)}}, \text{ as } x \to 0; \qquad (5)$$

in agreement with NBS # (7.1.5).

③ QM system of m_1 & m_2: express total $\hat{\mathbb{P}}$, $\hat{\mathbb{L}}$ & $\hat{\mathbb{K}}$ in cds $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ & $\mathbb{R}_{cm}$.

1) The CM transformation and its inverse are (w/ $M = m_1 + m_2$):



$$\left[\begin{aligned} \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2, \\ \mathbb{R} &= \frac{1}{M}(m_1\mathbf{r}_1 + m_2\mathbf{r}_2); \end{aligned}\right\} \leftrightarrow \left\{ \begin{aligned} \mathbf{r}_1 &= \mathbb{R} + (m_2/M)\mathbf{r}, \\ \mathbf{r}_2 &= \mathbb{R} - (m_1/M)\mathbf{r}. \end{aligned}\right. \qquad (1)$$

Symbolically: $\frac{\partial}{\partial \mathbf{r}_1} = \left(\frac{\partial \mathbf{r}}{\partial \mathbf{r}_1}\right)\frac{\partial}{\partial \mathbf{r}} + \left(\frac{\partial \mathbb{R}}{\partial \mathbf{r}_1}\right)\frac{\partial}{\partial \mathbb{R}} = \frac{\partial}{\partial \mathbf{r}} + \left(\frac{m_1}{M}\right)\frac{\partial}{\partial \mathbb{R}}$, i.e. $\nabla_1 = \nabla_r + \left(\frac{m_1}{M}\right)\nabla_R$; this works component-by-component. Treating $\partial/\partial\mathbf{r}_2$ similarly, we can write...

$$\rightarrow \nabla_1 = +\nabla_r + (m_1/M)\nabla_R, \quad \nabla_2 = -\nabla_r + (m_2/M)\nabla_R. \qquad (2)$$

2) The total system momentum is just that of the CM, since...

$$\hat{\mathbb{P}} = \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2 = -i\hbar(\nabla_1 + \nabla_2) = -i\hbar\left(\frac{m_1+m_2}{M}\right)\nabla_R = \underline{\underline{-i\hbar\nabla_R}}. \qquad (3)$$

The total system $\measuredangle$ momentum is that of the CM (about origin) plus that of the particles about the CM, since...

$$\hat{\mathbb{L}} = \hat{\mathbb{L}}_1 + \hat{\mathbb{L}}_2 = \mathbf{r}_1 \times \hat{\mathbf{p}}_1 + \mathbf{r}_2 \times \hat{\mathbf{p}}_2$$

$$= -i\hbar\left\{\left(\mathbb{R} + \frac{m_2}{M}\mathbf{r}\right)\times\left(\nabla_r + \frac{m_1}{M}\nabla_R\right) + \left(\mathbb{R} - \frac{m_1}{M}\mathbf{r}\right)\times\left(-\nabla_r + \frac{m_2}{M}\nabla_R\right)\right\}$$

$$\hat{\mathbb{L}} = \underline{\underline{-i\hbar\{\mathbb{R}\times\nabla_R + \mathbf{r}\times\nabla_r\}}} = \mathbb{R}\times\hat{\mathbb{P}} + \mathbf{r}\times\hat{\mathbf{p}} \quad \begin{cases} \mathbb{P} = -i\hbar\nabla_R, \text{ CM}; \\ \mathbf{p} = -i\hbar\nabla_r, \text{ relative.} \end{cases} \qquad (4)$$

This is just what happens in the CM transform of classical mechanics.

3) The kinetic energy operator transforms as...

$$\hat{\mathbb{K}} = \frac{1}{2m_1}\hat{\mathbf{p}}_1^2 + \frac{1}{2m_2}\hat{\mathbf{p}}_2^2 = -\frac{\hbar^2}{2}\left\{\frac{1}{m_1}\left(\nabla_r + \frac{m_1}{M}\nabla_R\right)^2 + \frac{1}{m_2}\left(\nabla_r - \frac{m_2}{M}\nabla_R\right)^2\right\}$$

cross-terms cancel

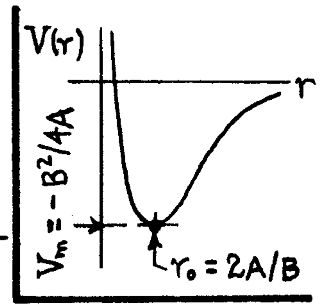
$$\text{So}\ \boxed{\hat{\mathbb{K}} = -(\hbar^2/2M)\nabla_R^2 - (\hbar^2/2\mu)\nabla_r^2} \quad \begin{cases} M = (m_1+m_2), \text{ total mass;} \\ \mu = m_1 m_2/(m_1+m_2), \text{ reduced mass.} \end{cases} \qquad (5)$$

As required. If the system Hamiltonian is: $\hat{\mathcal{H}} = \hat{\mathbb{K}} + V(r)$, where the interaction potential $V(r)$ depends on the relative cd $r = |\mathbf{r}_1 - \mathbf{r}_2|$, then we have shown: $\hat{\mathcal{H}} = \hat{\mathcal{H}}_{cm} + \hat{\mathcal{H}}_{rel}$, w/ $\hat{\mathcal{H}}_{cm} = -(\hbar^2/2M)\nabla_R^2$ is the free motion of the CM, and $\hat{\mathcal{H}}_{rel} = -(\hbar^2/2\mu)\nabla_r^2 + V(r)$ is the interaction in relative cds.

ϕ507 Solutions

④ [15 pts]. QM energy levels for central potential: $V(r) = -B/r + A/r^2$.

(A) 1) $V(r)$ vs. r is sketched at right. It has a minimum @ $r = r_0$ as shown ($V_{min} = -B^2/4A$ @ $r_0 = 2A/B$), and in a general way it resembles a molecular binding potential [Davydov ¶130].



(B) 2) Put $V(r)$ into the radial eqtn [Davydov Eq. (38.2)] to get...

$$\rightarrow \left\{\frac{d^2}{dr^2} + \left[\frac{2mE}{\hbar^2} + \frac{2m}{\hbar^2}\left(\frac{B}{r} - \frac{A}{r^2}\right) - \frac{l(l+1)}{r^2}\right]\right\} R(r) = 0. \tag{1}$$

The term in A can be combined with the term in $l(l+1)$ by defining...

$$\rightarrow \lambda(\lambda+1) = l(l+1) + 2mA/\hbar^2 \Rightarrow \underline{\underline{\lambda}} = \frac{1}{2}\left\{\left[(2l+1)^2 + \frac{8mA}{\hbar^2}\right]^{1/2} - 1\right\}. \tag{2}$$

We still have $l = 0, 1, 2, \ldots$, but $\lambda \neq$ integer $[\lambda \simeq l + (mA/(l+\frac{1}{2})\hbar^2)$, to $O(A)]$.

Eq. (1) is now a hydrogen-atom problem, with λ replacing l, viz...

$$\rightarrow \left\{\frac{d^2}{dr^2} + \left[\frac{2mE}{\hbar^2} + \frac{2mB}{\hbar^2}\frac{1}{r} - \frac{\lambda(\lambda+1)}{r^2}\right]\right\} R(r) = 0. \tag{3}$$

$$\left[\begin{array}{l} \ldots \text{atomic units}\} \text{ LENGTH}: \underline{\underline{a_0}} = \hbar^2/mB, \text{ ENERGY}: \underline{E_0} = B/a_0; \\ \ldots \text{dimensionless variables}\} \ \rho = r/a_0,\ \epsilon = E/E_0;\ \text{let } \epsilon = -\frac{1}{2}\kappa^2 \text{ for boundstates.} \end{array}\right] \tag{4}$$

Eq. (3), in these units, is converted to...

$$\rightarrow \left\{\frac{d^2}{d\rho^2} - \kappa^2 + \frac{2}{\rho} - \frac{\lambda(\lambda+1)}{\rho^2}\right\} R(\rho) = 0, \Rightarrow R(\rho) \sim \begin{cases} \rho^{\lambda+1}, & \text{as } \rho \to 0, \\ e^{-\kappa\rho}, & \text{as } \rho \to \infty. \end{cases} \tag{5}$$

3) As with the H-atom, extract the asymptotics by setting: $R(\rho) = \rho^{\lambda+1} e^{-\kappa\rho} f(\rho)$, so

$$\rightarrow z\frac{d^2 f}{dz^2} + (b - z)\frac{df}{dz} - af = 0, \text{ w/ } z = 2\kappa\rho,\ b = 2(\lambda+1),\ a = \lambda + 1 - \frac{1}{\kappa}. \tag{6}$$

This is a confluent hypergeometric eqtn, with solution: $f(\rho) = F(a; b; z)$.

$f(\rho)$ will diverge $\sim e^z = e^{2\kappa\rho}$ as $\rho \to \infty$ unless $a = -N$, where $N = 0, 1, 2, \ldots$; in that case, $f(\rho) \sim$ polynomial of degree N, and $R(\rho)$ is well-behaved as $\rho \to \infty$.

The condition $a = \lambda + 1 - \frac{1}{\kappa} = -N$ gives $\kappa = 1/(N + \lambda + 1)$, or -- for the energies:

$$E = -\tfrac{1}{2}E_0 k^2 = -\tfrac{1}{2}E_0/(N+\lambda+1)^2. \tag{7}$$

Write in the principal quantum # $n = N+l+1$; then the energies are

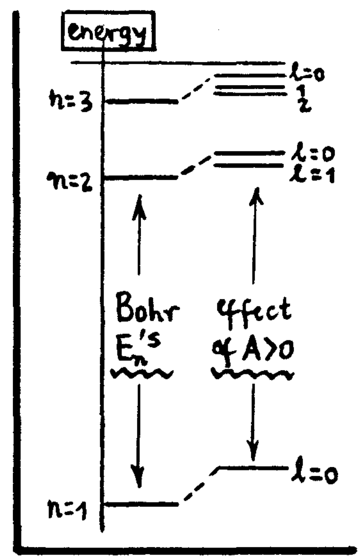
$$\boxed{E_{nl} = -\tfrac{1}{2}E_0/(n+\Delta_l)^2}, \text{ w/ } \underline{\underline{\Delta_l}} = \lambda - l = (l+\tfrac{1}{2})\left\{\left[1+\frac{2mA/\hbar^2}{(l+1/2)^2}\right]^{1/2}-1\right\}. \tag{8}$$

This expression is <u>exact</u> for the problem, and here $n=1,2,3,\ldots$, $l=0,1,\ldots,n-1$ in the usual fashion. So long as $A \neq 0$, the energies depend on l as well as n, so <u>the l-degeneracy peculiar to the H-atom is lifted by $A \neq 0$.</u>

(C) 4) If $|A| \to 0$, the "quantum defect" $\Delta_l \simeq mA/\hbar^2(l+\frac{1}{2})$ is small, and we can expand E_{nl} of Eq. (8). To first order in A, we get...

$$\left[\!\left[E_{nl} = -\frac{1}{2}\left(\frac{E_0}{n^2}\right)\Big/\left(1+\frac{\Delta_l}{n}\right)^2 \simeq -\left(\frac{E_0}{2n^2}\right)\left[1-\frac{4mA/\hbar^2}{(2l+1)n}\right]\right. . \tag{9}$$

The factor out in front, viz $-E_0/2n^2$, is the Bohr energy. But each Bohr level n now <u>splits</u> into n levels, with distinct energies for each of $l=0,1,\ldots,n-1$. For $A>0$, all the l-levels are lifted, with the $l=0$ (S-state) lifted most, and the $l=n-1$ state lying closest (but still above) to the original Bohr level; the $A>0$ case is sketched at right.



5) The "fine structure" created by $A>0$, for each n, is the $l=0 \to (n-1)$ multiplet width, viz.

$$\rightarrow \Delta E_n = E_{n,l=0} - E_{n,l=n-1} = \left(\frac{E_0}{n^3}\right)\frac{2mA}{\hbar^2}\left[1-\frac{1}{2n-1}\right]. \tag{10}$$

This ΔE_n shares at least feature in common with actual hydrogenic fine structure: there is <u>no</u> splitting in the ground state ($n=1$), and -- for larger n -- the splitting goes as $(1/n^3)$, roughly.