- yb22 file
- 5 [15pts]. This problem concerns details of H-atom radial wavefons in Davydor 9 38.
- A) When a = -N,  $^{W}N = 0, 1, 2, ...$ , show that the Confluent hypergeometric for F(a;b;x) reduces to the polynomial:  $F(-N;b;x) = \sum_{k=0}^{N} \frac{\Gamma(b)}{\Gamma(k+b)} \binom{N}{k} (-x)^k$ ,  $^{W}(N) = \frac{N!}{k!(N-k)!}$  the binomial coefficient. Using this result, find an explicit form for the full H-atom radial wavefern fre( $\rho$ ) =  $\frac{1}{\rho}$  Rne( $\rho$ ) for the 3s state. Compare with Davydor Table 8.
- (B) H-atom states  $|nl\rangle$  with maximum allowed 4 momentum l=n-1 are called "raster" states. Find the general form of the full radial wavefor fre(p) when l=n-1.
- (C) Calculate expectation values of powers of p, viz.  $\langle p^{\lambda} \rangle$ , in the states  $|n,l=n-1\rangle$  you found in part (B). For  $\lambda=-3$ , specifically, compare with Davydov's Eq. 38.17e.
- **6** A QM & momentum  $\hat{J}$  has eigenfons  $|z_m\rangle$ . Consider the ladder operators  $\hat{J}_{\pm}=\hat{J}_x\pm i\hat{J}_y$ . (A) Show that  $\hat{J}_{\pm}|z_m\rangle$  is an eigenfon of  $\hat{J}^2$ , with  $z_{\pm}$  value unchanged.
  - (B) Show that  $\hat{J}_{\pm}|_{Jm}$  is an eigenfer of  $\hat{J}_{z}$ , corresponding to eigenvalues  $m\pm 1$ .
  - (C) Using the  $\hat{J}_{\pm}$ , find the most general metrix elements of  $\hat{J}_{x} \notin \hat{J}_{y}$  i.e. evaluate  $\langle \alpha' j'm' | \hat{J}_{x,y} | djm \rangle$ , with pertinent selection rules for the quantum #5  $\alpha \alpha', jj', mm'$ .
- Floorsider the Pauli matrices  $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  for spin  $\frac{1}{2}$ ; they obey the commutation of xyz [Sakurai, Sec 3.2].
  - (A) Prove the anti-commutation rule: {  $\sigma_{\alpha}$ ,  $\sigma_{\beta}$ } =  $\sigma_{\alpha}\sigma_{\beta} + \sigma_{\beta}\sigma_{\alpha} = 2\delta_{\alpha\beta}$ .
  - (B) If  $\vec{A} \in \vec{B}$  are any two vector operators that commute with  $\vec{\sigma}$ , use  $[\sigma_{\alpha}, \sigma_{\beta}]$  and  $[\sigma_{\alpha}, \sigma_{\beta}]$  to prove the Dirac identity:  $(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = \vec{A} \cdot \vec{B} + i \vec{\sigma} \cdot (\vec{A} \times \vec{B})$ .
- B If vector operators  $\vec{A} \neq \vec{B}$  are both  $\vec{T}$ -vectors W.r.t. a QM & momentum operator  $\vec{J}$ , Show that:  $[\vec{J}, \vec{A} \cdot \vec{B}] = 0$ . Why does this establish  $\vec{A} \cdot \vec{B}$  as a true scalar"?
- $\exists$  [5pts]. Given: noncommuting operators  $\hat{P} \in \hat{Q}$  and a set of basis fons {uk(x)}. If  $Pij = \int dx \ u_i^*(x) \hat{P} \ u_j(x)$ , verify the matrix egth:  $(PQ)_{ke} = \sum_{m} P_{km} \ Q_{me}$ , directly. What assumption(s) must be made about the set {uk(x)}?

[5[15pts]. Explore details of H-atom radial wavefens in Davydor 938.

(A)  $F(a;b;x) = \sum_{k=0}^{\infty} [(a)_k/(b)_k] \frac{x^k}{k!}$ , and with  $|a|_k = \Gamma(k+a)/\Gamma(a)$ , we can write:

$$\rightarrow F(-N;b;x) = \sum_{k=0}^{\infty} \frac{\Gamma(b)}{\Gamma(k+b)} \left[ \frac{\Gamma(k-N)}{\Gamma(-N)} \right] \frac{x^k}{k!} , N=0,1,2,...$$

We must deal with the [].  $\Gamma(z)$  diverges at z=(-1)N, and so the []=0 for all k>N. This means the series <u>terminates</u> at k=N. For  $0 \le k \le N$ , the [] is of indeterminate form  $\pm \infty/\infty$ . But from the reflection formula for  $\Gamma$ -fors [see NBS Handbook # (6.1.17)]:  $\Gamma(z)\Gamma(1-z) = \pi \csc \pi z$ , it is easy to show...

Thus, except for sign, (-)<sup>n</sup>,  $\Gamma(z)$  diverges in the same way (namely as  $\frac{1}{E}$ ) when  $z \to -n$ , any (-)ve integer. If  $m \nmid n$  are integers:  $m! \Gamma(-m)/n! \Gamma(-n) = (-)^{m-n}$ , is finite. Applying this result to Eq. (1)...

$$\left[\frac{\Gamma(k-N)}{\Gamma(-N)}\right] = (-)^k \frac{N!}{(N-k)!} \Rightarrow F(-N;b;x) = \sum_{k=0}^N \frac{\Gamma(b)}{\Gamma(k+b)} \binom{N}{k} (-x)^k \ . \tag{3}$$

 $\binom{N}{k} = \frac{N!}{k!} (N-k)!$  is the binomial coefficient. <u>NOTE</u>: this result can be gotten also by using Leibniz' formula to differentiate the definition of the Laguerre polynomial  $L_N^{b-1}(x)$  associated with F(-N;b;x) [Dayydov, Math. App. D, Eqs. (D7) & (D8)].

In his Eq. (38.16), Davydor writes the full FI-atom radial wave for as ...

For the 3s state,  $n=3 \notin l=0$ , so  $N=2 \notin b=2$ . Then  $N_{30}=\frac{1}{\sqrt{2}}(2\mathbb{Z}/3)^{\frac{3}{2}}$ , and  $\chi=\frac{2}{3}\mathbb{Z}\rho$ . Also [by Eq.(3)]:  $F(-N;b;x)=F(-2;2;x)=1-x+\frac{1}{6}x^2$ . Then have:

$$f_{30}(p) = N_{30}F(-2;2;x)e^{-x/2} = \frac{2z^{3/2}}{3\sqrt{3}}\left[1-\frac{2}{3}Zp+\frac{2}{27}(Zp)^2\right]e^{-\frac{1}{3}Zp}$$

This agrees with the 35 entry in Davydov's Table 8 when 2=1 (hydrogen).

(B) For the "raster" states  $|n,l=n-1\rangle$ , the radial quantum # N=n-(l+1)=0, and—by Eq.(3)—have  $F(0;b;x)\equiv 1$ . By Eq.(4), the radial wave fens reduce to  $\frac{f_{n,n-1}(p)}{n}=N_{n,n-1}\frac{x^{n-1}}{n}e^{-x/2}$ ,  $x_{n}=\frac{2zp}{n}$ ,  $N_{n,n-1}=\left(\frac{zz}{n}\right)^{\frac{3}{2}}\sqrt{\frac{1}{(2n)!}}$ .

(C) The expectation value of p2 in the rester state of Eq. (6) is...

$$\rightarrow \langle \rho^{\lambda} \rangle = \int_{0}^{\infty} f_{n,n-1}^{*}(\rho) \left[ \rho^{\lambda} \right] f_{n,n-1}(\rho) \cdot \rho^{2} d\rho = \int_{0}^{\infty} d\rho \, \rho^{\lambda+2} \left[ f_{n,n-1}(\rho) \right]^{2}.$$

The  $\chi$  har integration  $\int_{4\pi} d\Omega |Y_{em}(\theta, \varphi)|^2 = 1$  has been done. With  $f_{n,n-1}(p)$  the real radial wovefor of Eq.(6)...

$$\langle \rho^{\lambda} \rangle = \frac{1}{(2n)!} \left( \frac{2Z}{n} \right)^{\frac{3}{2}} \int_{0}^{\infty} d\rho \, \rho^{\lambda+2} \, \chi^{2n-2} \, e^{-\chi}, \quad \chi = (2Z/n) \rho$$

$$= \frac{1}{(2n)!} \left( \frac{n}{2Z} \right)^{\lambda} \int_{0}^{\infty} d\chi \, \chi^{2n+\lambda} \, e^{-\chi} \leftarrow \text{tabulated integral [e.g. Dwight # (860.07)]}$$

$$\langle \rho^{\lambda} \rangle = \left(\frac{n}{27}\right)^{\lambda} \frac{\Gamma(2n+\lambda+1)}{(2n)!}; \quad \langle \rho^{\lambda} \rangle = \left(\frac{n}{27}\right)^{\lambda} \frac{(2n+\lambda)!}{(2n)!}, \quad \forall \lambda = \text{integer}. \quad (8)$$

For λ=-3, Eq. (8) gives...

$$\left\langle \frac{1}{\rho^{3}} \right\rangle = \left( \frac{n}{2Z} \right)^{-3} \frac{(2n-3)!}{(2n)!} = \left( \frac{2Z}{n} \right)^{3} / 2n(2n-1)(2n-2)$$

$$\int_{0}^{\infty} \left( \frac{1}{\rho^{3}} \right) = \left( \frac{Z}{n} \right)^{3} / n(n-\frac{1}{2})(n-1) = \left( \frac{Z}{n} \right)^{3} / (l+1)(l+\frac{1}{2}) l, \quad \text{where } l=n-1.$$
(9)

Our result for (1/p3) agrees with Davydov's Eq. (38.17e) in the case we are con-Sidering, viz. 1=n-1. Similarly, Eq. (8) gives, with 1=n-1 properly inserted

$$\langle 1/p^2 \rangle = \left(\frac{Z}{n}\right)^2/n (n - \frac{1}{2}) = \frac{Z^2}{n^3}/(l + \frac{1}{2}) \iff \text{Davydov Eq.}(38.17d)$$
  
 $\langle 1/p \rangle = Z/n^2 \quad (\text{no } l - \text{dependence}) \iff \text{u} \quad \text{u} \quad (38.17c)$   
 $\langle p \rangle = \frac{n}{Z} (n + \frac{1}{2}) = \frac{3n^2 - l(l + 1)}{2Z} \Big|_{l=n-1} \iff \text{u} \quad (38.17a).$ 

6 Elementary operations with & momentum ladder operators J± [Sakurai, Sec. 3.5].

(A)  $\hat{J}^2$  commutes with every one of the components  $\hat{J}_k$  of  $\hat{J}$ , i.e.  $[\hat{J}^2, \hat{J}_k] = 0$ , where k = x, y, z [Sakurai, Eq. (3.5.2)]. So, obviously  $[\hat{J}^2, \hat{J}_{\pm}] = 0$ . Now consider  $\Psi =$ Igm) an eigenfon of  $\hat{J}^2$ , i.e.  $\hat{J}^2\psi = g(y+1)\psi$ . Let  $\phi_{\pm} = \hat{J}_{\pm}\psi$ , and look at

 $\rightarrow \hat{J}^2 \phi_{\pm} = \hat{J}^2 \hat{J}_{\pm} \psi = \hat{J}_{\pm} \hat{J}^2 \psi = 3(3+1) \hat{J}_{\pm} \psi = 3(3+1) \phi_{\pm}.$ 

So, as required,  $\phi_{\pm} = \hat{J}_{\pm} |_{Jm}$  is an eigenfon of  $\hat{J}^2$  with j unchanged.

(B)  $\Psi = |jm\rangle$  is an eigenfen of  $\hat{J}_{z}$ , i.e.  $\hat{J}_{z}\Psi = m\Psi$ . Now consider  $\hat{J}_{z}\phi_{\pm}$ , where (as above)  $\phi_{\pm} = \hat{J}_{\pm} \psi$ . By adding & subtracting  $\hat{J}_{\pm} \hat{J}_{z}$ , we can write ...

 $\rightarrow \hat{J}_{z} \phi_{\pm} = \hat{J}_{\bar{z}} \hat{J}_{\pm} \psi = \hat{J}_{\pm} \hat{J}_{\bar{z}} \psi + [\hat{J}_{\bar{z}}, \hat{J}_{\pm}] \psi.$ 

The first term RHS is just mot. As for the second term RHS, calculate

 $\left[ \left[ \hat{J}_{2}, \hat{J}_{\pm} \right] = \pm \hat{J}_{\pm} \leftarrow \text{Sakurai Eq. (3.5.6b)} \left[ \text{use of } \left[ \hat{J}_{\alpha}, \hat{J}_{\beta} \right] = i \hat{J}_{\gamma}, \text{etc.} \right] \cdot \left( \frac{3}{2} \right) \right]$ 

Eq. (2) =>  $\hat{J}_2 \phi_{\pm} = (m \pm 1) \phi_{\pm}$ (4)

As required,  $\phi_{\pm} = \hat{J}_{\pm} |_{2m}$  is an eigenfon of  $\hat{J}_{z}$  with eigenvalue  $m\pm 1$ .

(C) We can express:  $\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$ , and  $\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$ , and we "know.".  $\hat{J}_{\pm} |\alpha_{3}m\rangle = \sqrt{(3 \mp m)(3 \pm m + 1)} |\alpha_{3} m \pm 1\rangle \leftarrow Sakurai Egs (3.5.39 \ 40). (5)$ 

The quantum #5 & (total & momentum) and a (all other quantum #5) remain un-Changed, and the matrix element (a'g'm'IIx |azm) = Saar Syr (aym'IIx |aym).

When we insert  $\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$ , this M.E. vanishes except when  $m' = m \pm 1$ . So...

 $\langle \alpha' j' m' | \hat{J}_{x} | \alpha_{j} m \rangle = \frac{1}{2} \delta_{\alpha \alpha'} \delta_{jj'} \begin{cases} \sqrt{(j-m)(j+m+1)}, & \text{when } m' = m+1; \\ \sqrt{(j+m)(j-m+1)}, & \text{when } m' = m-1. \end{cases}$ Selection:  $\Delta \alpha = 0$ ,  $\Delta J = 0$ ,  $\Delta m = \pm 1$ 

 $\langle \alpha' j' m' | \hat{J}_{y} | \alpha_{j} m \rangle = \frac{1}{2i} \delta_{\alpha \alpha'} \delta_{jj'} \left\{ \frac{\sqrt{(j-m)(j+m+1)}}{(-1)\sqrt{(j+m)(j-m+1)}}, \text{ when } m' = m+1; \right\}$ 

(6b)

(6a)

(3) Carry out manipulations with the Pauli matrices of for spin 1/2.

(A) From the explicit representation:  $(\sigma_x, \sigma_y, \sigma_z) = (\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}) -- see$ Sakurai, Eq. (3.2.32) =- we verify directly that:  $\sigma_x^2 = \binom{01}{10}\binom{01}{10} = \binom{10}{10} = 1$ . Also,  $\sigma_y^2 = 1 \notin \sigma_z^2 = 1$ , similarly. Thus  $\sigma_x^2 = 1$  for each of  $\alpha = x, y, z$ .

For d + B, again look at explicit forms ...

So: JaJp+JBJa=0, when a \$ B. Combined with Ja=1, we get

$$\{\sigma_{\alpha}, \sigma_{\beta}\} = \sigma_{\alpha}\sigma_{\beta} + \sigma_{\beta}\sigma_{\alpha} = 2\delta_{\alpha\beta}$$
, (2)

which is the desired anticommutation rule.

(B) If we just add the equations 
$$\{\sigma_{\alpha}, \sigma_{\beta}\} = 2\delta_{\alpha\beta}$$
 and  $[\sigma_{\alpha}, \sigma_{\beta}] = 2i\epsilon_{\alpha\beta\gamma}\sigma_{\gamma}$ , then   
 $\rightarrow \sigma_{\alpha}\sigma_{\beta} = \delta_{\alpha\beta} + i\epsilon_{\alpha\beta\gamma}\sigma_{\gamma}$   $\int_{-\infty}^{\infty} \epsilon_{\alpha\beta\gamma} = \{\pm 1, \text{ for } \alpha\beta\gamma = \{\text{even}\} \text{ perm}^{n} \text{ of } xyz; \{3\}$ 

Then the Dirac identity is easy ...

Then the Durke laterting is easy...

$$\frac{(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B})}{(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B})} = \sum_{\alpha,\beta} (\sigma_{\alpha} A_{\alpha})(\sigma_{\beta} B_{\beta}) = \sum_{\alpha,\beta} (\sigma_{\alpha} \sigma_{\beta})(A_{\alpha} B_{\beta})$$

$$= \sum_{\alpha,\beta} (\delta_{\alpha\beta} + i \epsilon_{\alpha\beta\gamma} \delta_{\gamma}) A_{\alpha} B_{\beta}$$

$$= \sum_{\alpha,\beta} (\delta_{\alpha\beta} + i \epsilon_{\alpha\beta\gamma} \delta_{\gamma}) A_{\alpha} B_{\beta}$$

$$= \sum_{\alpha,\beta} (\delta_{\alpha\beta} + i \epsilon_{\alpha\beta\gamma} \delta_{\gamma}) A_{\alpha} B_{\beta}$$

$$= \sum_{\alpha,\beta} (A_{\alpha} B_{\alpha} + i \sum_{\alpha,\beta} \sigma_{\gamma} (\epsilon_{\alpha\beta\gamma} A_{\alpha} B_{\beta})$$

$$= A_{\alpha} B_{\beta} + i \sigma_{\alpha} (A_{\alpha} B_{\beta}).$$

$$= A_{\alpha} B_{\beta} + i \sigma_{\alpha} (A_{\alpha} B_{\beta}).$$

$$(4)$$

## REMARKS

1. Sakurai proves the Dirac identity in his Eq. (3.2.40).

2. For of's for spin 1 & spin 3/2, see Schiff "QM" (3rd ed., 1968), Sec. 27. NOTE: the relation {  $\sigma_{\alpha}, \sigma_{\beta}$  } = 28 as is obeyed only for spin 1/2.

8 Show that [J, A.B]=0, for A&B as T-vectors w.r.t. J.

Consider the & component of the commutator. It can be written as ...

$$\longrightarrow [\vec{J}, \vec{A} \cdot \vec{B}]_{\alpha} = \sum_{\beta} [J_{\alpha}, A_{\beta} B_{\beta}] = \sum_{\beta} \{A_{\beta} [J_{\alpha}, B_{\beta}] + [J_{\alpha}, A_{\beta}] B_{\beta}\}. \quad (!)$$

We have used the commutator identity: [P,QR] = Q[P,R]+[P,Q]R. Since  $\vec{A} \not= \vec{B}$  are both  $\vec{T}$ -vectors w.r.t.  $\vec{J}$ , then in Eq.(1) we can set...

$$\begin{array}{l}
\stackrel{\text{Sol}}{\longrightarrow} \left[ \overrightarrow{J}, \overrightarrow{A} \cdot \overrightarrow{B} \right]_{\alpha} = i \sum_{\beta, \gamma} \varepsilon_{\alpha\beta\gamma} \left\{ A_{\beta} B_{\gamma} + A_{\gamma} B_{\beta} \right\} \\
= i \left\{ \sum_{\beta, \gamma} \varepsilon_{\alpha\beta\gamma} A_{\beta} B_{\gamma} - \sum_{\gamma, \beta} \varepsilon_{\alpha\gamma\beta} A_{\gamma} B_{\beta} \right\}.
\end{array}$$
(3)

Each term on RHS of Eq. (3) is equivalent to  $(\vec{A} \times \vec{B})_{\alpha}$ . So, as required...

$$[\vec{J}, \vec{A} \cdot \vec{B}] = i \{ (\vec{A} \times \vec{B}) - (\vec{A} \times \vec{B}) \} = 0.$$

This result is independent of whether  $\vec{A} \notin \vec{B}$  commute with each other.

Under the ossmal rotation operator (rotation by 4 89 about axis n), viz.  $R(\delta \varphi) = 1 - i \delta \varphi(\hat{n} \cdot \hat{J}), [Sakurai Eq.(3.1.15)], a scalar S transforms as$ 

$$\begin{bmatrix} S \to S' = R^{-1}SR = S + i \delta \varphi [\hat{n} \cdot \vec{f}, S], & 1^{12} \text{ orden in } \delta \varphi; \\ {}^{3}V \delta S = S' - S = i \delta \varphi [\hat{n} \cdot \vec{f}, S].
\end{bmatrix}$$
(5)

If S is a "true scalar", it will be unaffected by such a rotation, i.e. 85=0. This requires  $[\hat{n}\cdot\hat{J},S]=0...$  or that S commute with each component of  $\bar{J}$ , i.e. [J,S]=0. Then S= A·B is a "true scalar" by virtue of Eq. (4).

<sup>\*</sup> Easy = ±1 if asy = { even} permutation of 123. Otherwise Easy = 0.

9[5pts]. Prove: (PQ)ke = 2 Pkm Qme W.n.t. basis {uk(x)}.

The RHS of the identity is

 $\longrightarrow \sum_{m} P_{km} Q_{me} = \sum_{m} \int dx \, u_{k}^{*}(x) \, \hat{P} \, u_{m}(x) \int dx' \, u_{m}^{*}(x') \, \hat{Q} \, u_{e}(x')$ 

=  $\int dx \, u_k^*(x) \, \hat{P} \int dx' \left[ \sum u_m(x) \, u_m^*(x') \right] \, \hat{Q} \, u_e(x')$ . (1)

But the "basis"  $\{u_k(x)\}$  is by assumption a <u>complete set</u> of fens on the (Common) domain of  $\hat{P} \not\in \hat{Q}$ . Such a complete set obey the closure relation:

 $\longrightarrow \sum_{m} u_{m}(x) u_{m}^{*}(x') = \delta(x-x'), Dwac delte fon.$ 

The [] in Eq. (1) can be replaced by the 8-for, and we have -- as desired

 $\begin{bmatrix}
\sum_{m} P_{km} Q_{me} = \int dx \, u_{k}^{*}(x) \, \hat{P} \int dx' \, \delta(x-x') \, \hat{Q} \, u_{k}(x') \\
= \int dx \, u_{k}^{*}(x) \, \hat{P} \, \hat{Q} \, u_{k}(x) = (PQ)_{ke} \, .
\end{bmatrix} \, \underbrace{QED}$ 

The <u>ordering</u> of PAQ has been respected, so the proof holds whether or not PAQ commute. One need only assume the {uk(x)} are a complete set.

In the language of boos and kets, the proof goes as ...

More efficient, but more abstract.