A Winter's Two-Day Walk through Saxon PhL 12.22.08

On that two-day walk, I skipped a few sections, then did them later.

About the Author and the Book 2
Chapter I: the Dual Nature of Matter and Radiation 3
1. Breakdown of Classical Physics 3
2. QM concepts like ψ, observables and uncertainty principle 4
3. Wave aspects of particles. 4
4. Numbers. 4
5. The particle aspects of waves. 4
Chapter II: State Functions and their Interpretation (18) 4
Chapter III. Linear Momentum (29) 5
1. The 1D Plane Wave Momentum Eigenstate. 5
2. Wave Packets. 5
3. Fourier and Delta Functions. 5
4. Momentum and "Configuration" Space 6
5. Momentum and Position Operators. 6
6. Commutation Relations(45) 6
7. The Uncertainty Principle 6
Chapter IV. Motion of a Free Particle (56) 6
1. Motion of a Wave Packet: Group Velocity. 6
2. Correspondence Principle at Work. 6
3. The free packet in x-space. 6
5. Gaussian packet moving in time. 7
6. The Free Particle SE (66). 7
7. Probability conservation. 7
8. Dirac Bracket Notation (72) 7
9. Stationary States. 7
11. Summary. Not bad. 7
Chapter V. Schrodinger's Equation (84) 8
1. Probability conservation. 8
2. Hermitian operators. 8
4. The SE in x-space and in p-space. 8
5. Stationary states. 8
6. Eigenfunctions and eigenvalues of Hermitian Operators. 8
7. Simultaneous Observables and Complete Sets of Operators. 8
Chapter VI. States of a Particle in 1D (116) 8
3. The Square Well (121). 9
4. The Harmonic Oscillator (126). 9
5. The Creation Operator Representation (138). 9
6. Packet in the HO potential (144) 9
7. Continuum States in a Square Well (147). 10
9. Wave packet passing through a potential. 10
10. Numeric Solution for Packet (158) 10
Chapter VII. Approximation Methods (174) 10

1. The WKB Approximation.....10
2. Rayleigh-Ritz variational method (184) 11
3. Stationary State Perturbation Theory (Non-Degenerate Case). (189).....12
4. Matrices.....14
5. Degenerate or Close-Lying States (p 204).....14
6. Time-dependent perturbation theory (and transition probability and golden rule) (208) 22
Chapter VIII. Systems of Particles in 1D (227) 22
1. Formulation.....22
2. Two particles and CMS (229).....23
3. Interacting particles under uniform external forces. 23
4. Coupled Harmonic Oscillators (236). 23
5. Weakly interacting particles with external forces. 23
6. Identical particles and exchange degeneracy. 23
7. Systems of two identical particles (243). 23
8. Many-particle systems and Pauli Principle.(245). 23
9. Systems of three identical particles.....23
10. Weakly interacting identical particles with external forces (255).....23
Chapter IX. Motion in three dimensions (262) 23
1. Formulation: motion of one free particle. 24
2. V(r) separable in Cartesian coordinates. 24
3. Central Potential: angular momentum eigenstates (268). 24
5. The H atom. 26
Chapter X. Angular Momentum and Spin (298).....26
1. Orbital L (298). 26
2. Eigenfunctions and eigenvalues.....26
3. Rotation and translation operators. 27
4. The Pauli Operators. 27
5. Adding Angular Momenta. 27
Chapter XI. Applications and Further Generalizations (344) 27
1. The Helium Atom and the Periodic Table. 27
2. Theory of Scattering. 28
3. The Born Approximation. 28
4. Motion in an EM Field. 28
5. The Dirac Theory of the Electron. 28
6. Mixed States and the Density Matrix.....28
Appendix I: Gaussian Integrals (397) 28
Appendix II: Selected References (400) 29

About the Author and the Book

Published Holden-Day in 1968. David S. Saxon, *Elementary Quantum Mechanics*. (mort 2005)

★★★★★ **Hitting the mark**, July 19, 2001

By **James M Lawler** (San Diego, CA United States) - See all my reviews

It's too bad this book went out of print. It is succinct and well written. It achieves the right level as a textbook for an undergraduate's first yearlong course in QM.

The book is sufficiently lucid that it can be used as a self-study textbook.

This 1968 book never had any future editions, and is no longer in print, used copies maybe $10 and up on the web. The author is dead, the book will probably just fade away into history.

Saxon used this book at UCLA for a 2 quarter *juniors* course (2/3rd of an academic year), the guy above mentions a year long course. Saxon's UCLA professor career ran 28 years 1947-1975 when he became President of the entire UC system for 8 years, then did similar for MIT till 1990, then I guess had a nice 15 years of retirement time before death arrived at age 85.

I used this book for independent study in the Fall Quarter of my *senior* Harvard year 1969. I was doing King on transmission lines, Op Amps with Roberge at MIT, and this and Feynman with Purcell as adviser. No formal classes at all! I remember well many long sessions at the Radcliffe Hillis library where I would hunker down in one of its perfectly lighted table/booth deals and spent hours on this book, coffee available on the top floor, got my mind off social matters for a while.

I have just "read" through most of this 400 page book in 2 days, with notes as below. My motivation at first was just to see what Saxon said about scattering, since I had just finished reading Schiff Chapter 5. But then I decided to just browse the entire book for old time's sake since I liked it so much in 1969.

David S. Saxon

From Wikipedia, the free encyclopedia

David S. Saxon (1920 – December 8, 2005) was an American physicist and educator who served as the President of the University of California system as well as the Chairman of the Board of Trustees of the Massachusetts Institute of Technology Corporation.

Saxon was born in St. Paul, Minnesota. He attended MIT where he earned a B.S. degree in 1941 and Ph.D. in 1944, both in Physics. He worked in MIT's famed wartime Radiation Laboratory during World War II.

Saxon joined UCLA in 1947, but was dismissed in 1950 with thirty other faculty members because of their objection to signing an oath of loyalty and declaration that they were not Communist Party members. The California Supreme Court later invalidated this requirement and Saxon returned to UCLA in 1952. While at UCLA, Saxon was a dean, vice chancellor, and executive vice chancellor. He served as the president of the University of California system between 1975 and 1983.

Saxon joined the MIT Corporation in 1977 and held the office of Chairman between 1983 and 1990.

Saxon was a Fellow of the American Academy of Arts and Sciences and a member of the American Philosophical Society, American Physical Society, and the American Association for the Advancement of Science.

Saxon was married to his wife, Shirley for 65 years and had six daughters and six grandchildren.

Jim Ball: B.S., 1956, California Institute of Technology (CalTech, not UCLA)
Ph.D., 1960, University of California (Berkeley)

Chapter I: the Dual Nature of Matter and Radiation

1. Breakdown of Classical Physics

2. QM concepts like ψ, observables and uncertainty principle

3. Wave aspects of particles. deBroglie $\lambda = h/p$. Davisson Germer 1927 diffraction. Saxon then presents two idealized 1D "experiments" to illustrate. The first is scattering against a finite-height potential wall, physically realized by two drift tubes. If you model this classically as a ball rolling up a rise, you would expect 100% transmission if ball energy is more than the height energy. The QM fact is that for energy below the wall height, you get 100% reflection as expected, but for energy a small amount above the wall, you do not get 100% transmission, you get some reflection. This goes away and becomes classical as E increases. in the second experiment, a third drift tube is added to make a potential "post". Saxon plots the transmission coefficient versus energy but does not do this calculation (yet), just imagines as with experiment #1 that we are seeing the "experimental results". We see **tunneling** at energy below the post top, and 100% transparency but with dips between at certain energies above the post, highly non-classical. Classically, we would expect just a box edge graph.

4. Numbers. QM characteristic numbers are **small**, hence we don't usually see QM effects in our world.

5. The particle aspects of waves. The **blackbody** catastrophe is outlined as embodied in Rayleigh-Jeans Law, and it is repaired by (1900 Planck) assuming $E = h\nu$ for an occupied mode, rather than $E = 1/2$ kT, suggesting the notion of a "photon" particle. In 1905 Einstein used this same assumption to explain photoelectric emission. In 1923 the energy loss in Compton scattering of photons off electrons also fit with the idea of light as photons.

6. Complementarity. The wave and particle nature are both right, and [wave, particle] ~ $\hbar$ says that some experiments see one nature and other experiments see the other nature. A second idea is that of ψ and probability, that measurement "**collapses**" the wavefunction into a 100% observed eigenvalue (cat is observed to be 100% dead or 100% alive). A third idea is that [experiment, observer] ~ $\hbar$ because the observer is part of ψ. It seems that Bohr and Heisenberg's names are associated with these general ideas, collectively known as the **Copenhagen Interpretation**, since these two collaborated at the University of Copenhagen in 1927. The Cat.

7. The Correspondence Principle. Hardly seems worthy of having a name, we know that any "quantum theory" must duplicate classical results in the appropriate limit. Of course this idea can rule out certain theories.

Saxon has done a good job with this chapter.

Chapter II: State Functions and their Interpretation (18)

Properties of ψ are discussed: **Superposition** causes **interference** just as with normal waves. **Probability** as $|\psi^2|$, and **normalization**. What equation determines ψ(x,t) (no answer yet)? **Expectation values** and **observation**. **Ehrenfest** says that classical laws like p = mv should become <p> = m<v> etc. Comparison of what a Gaussian **wave packet** does classically and in QM: in QM the width increases, but don't see in macro world. I don't see in a cursory scan any mention about ψ being a complex valued function, but we do of course see $|\psi^2|$ which implies ψ might be complex.

I am sure this chapter is here because students Saxon dealt with had trouble with these concepts. Perhaps earlier courses just got on with the SE with no comments about ψ.

Chapter III. Linear Momentum (29)

1. The 1D Plane Wave Momentum Eigenstate. Here it is in all its glory, and yes, it is complex. Saxon aptly states that once you accept this plane-wave form as a travelling-wave complex phasor representing a state of definite momentum p or k, the "**QM rabbit is already in the hat**". Almost all else really follows from this phasor assumption. Since it is a phasor, $|\psi^2| = 1$ so probability of being anywhere is the same, so we have a full illustration of $[\Delta p, \Delta x] \sim \hbar$. Either idea implies the other for a plane wave. So perhaps this is some motivation for ψ being in general complex. I remember having trouble accepting this plane wave thing in 1969.

2. Wave Packets. Just linearly combine these plane waves to make packets, $\psi = \int dp \text{ plane } \varphi(p)$, allowed superposition idea. Then φ(p) is the momentum-space wavefunction. You can then compute the value of ψ(x,t) from ψ(x,0) if you know φ(p). **Fourier** stuff. A φ(p) box of half-width Δp gives the usual sinc function in x, probably this was one of the first times I saw this happening. Fourier was all new to me at this time.

3. Fourier and Delta Functions. Saxon starts with f(θ) as a sum of $e^{in\theta}$, not an integral, n = integer. Then f_n he calls A_n is integral of f, and this is Fourier Series. Changes θ = πx/L. Takes a limit, and we end up with the Fourier Integral transform (11) page 35 where he spreads out the 2π evenly. At this point in my physics life, I had probably learned about Fourier Series, so this integral transform was new. This then implies the usual expo representation of the delta function (13), and the usual **"delta rules"** are listed off on page 37.

He then quotes the **"convolution theorem"** which says the FT of a product of functions can be written as a convolution integral of their transforms. A special case is **Parseval's Theorem** which really says to me that the FT is a unitary transformation, and obviously if $M_{tk} = e^{-ikt}$, then $M^{-1} = M^{\dagger}$.

What Saxon does not say is that if you have an equation $g_3(k)$ = convolution integral of $g_1(k)$ and $g_2(k)$, then in x-space you will find that $G_3(x) = G_1(x)\, G_2(x)$ and you have simplified things a lot because you have gotten rid of an integral. Think of it this way:

$$(g_3)_k = \Sigma_{k'}(g_2)_{k-k'}\,(g_1)_{k'} = \Sigma_{k'}[K_{k,k'}]\,(g_1)_{k'} \qquad \text{or the matrix equation } g_3 = K\, g_1$$

where the matrix $K_{k,k'} = (g_2)_{k-k'}$ is non-diagonal. Then in x-space think

$$(G_3)_x = (G_2)_x\,(G_1)_x = \Sigma_{x'}\,[\delta_{x',x}\,(G_2)_x]\,(G_1)_x \quad \text{or the matrix equation } G_3 = \Lambda\, G_1$$

where the matrix $\Lambda_{x',x} = [\delta_{x',x}\,(G_2)_x]$ *is* diagonal. Thus, you can **diagonalize a matrix equation** of convolution time by doing a FT. Saxon's book is 1968, I am not sure how widespread the FT was in EE texts at that time, a full 40 years ago.

Fourier Series were done by **Fourier in 1807.** I am unable to determine who first applied this to non-periodic functions and talked about both sides being an integral, perhaps it was Fourier at the same time. He was studying **heat**, and the idea that a function was a sum of sines was not well accepted.

4. Momentum and "Configuration" Space.

5. Momentum and Position Operators. By looking at <p> in p-space, then transforming to x-space, you find that for an arbitrary state ψ we must have $p = -i\hbar\partial_x$ as the operator which represents "p" in x-space, and vice versa with the opposite sign. Saxon then backs out a bit and talks about **linear operators** in general and how they don't in general commute

6. Commutation Relations(45). We first learn that $[p,x] = -i\hbar$ and then $[p,f(x)] = -i\hbar f'(x)$ which I would show from parts integration somehow.

7. The Uncertainty Principle. We first look at the square wave ψ in x-space, compute the sinc, and examine the Δx and Δp situation to find that the product is $\sim \hbar$. Second we look at a Gaussian $\psi(x)$ and arrive at the same conclusion, for these two very different but fairly smooth functions. For messy functions, we expect to find that $\Delta x\ \Delta p > \hbar$. For me, all this just comes from the Fourier integral transform. Once you accept that, you get the UP. This then applies to any Fourier pair of coordinates.

So the UP is "built into QM" as he says. You can use the UP to predict general things, and we have three examples. (1) the angle of diffraction through a slit (2) resolution of a microscope re λ light (3) the best example: If a particle is in some region a, you can compute Δp and hence KE and hence E as the general function shown in (58). You can minimize E to find a. For H atom, doing this gives Bohr radius, so you learn a lot by doing hardly anything! You have really shown that a ground state must exist otherwise you violate UP, and this explains why the H atom does not collapse, ie, why there is a "ground" state. Very good Mr. Saxon.

Chapter IV. Motion of a Free Particle (56)

1. Motion of a Wave Packet: Group Velocity. Make a packet with a narrow spread Δp in momentum space, expand k or $\omega(p)$ as Taylor series, keep first term, compute what an initial packet does, and you find it moves undistorted for a certain time with group velocity $v_g = \hbar\,\omega'(p)$. This $\omega(p)$ thing is what appears in page 56 (1). For a free non-rel particle, I know that $\hbar\omega = E = p^2/2m$ so $\omega(p) = p^2/2m\hbar$ and $\omega'(p) = p/m\hbar = v/\hbar$ so $v_g = v$. The time limit is shown in (6) page 59 in terms of $\omega''(p) = 1/m\hbar$ and the original Δp of the packet

2. Correspondence Principle at Work. By treating $\omega(p)$ as unknown, and insisting that $v_g = v$, we can conclude backwards that $p^2/2m = \hbar\omega$. So just our assumptions so far (no SE yet) tell us $\lambda = h/p$ so we have now "derived" this thing that Planck used to fix the blackbody problem. He then looks at the time required for a 1 gram packet of size 1 micron to start spreading and gets the age of the universe.

3. The free packet in x-space. We know what this looks like as an integral of plane waves. We then show that we can get $\psi(x,t)$ from $\psi(x',0)$ via the kernel (of a dx' integral) he calls $K(x',x,t)$ which kernel is then a certain phasor integral. We are then referred to **Appendix I** (just as I would have done!) to state the result as a closed form expression. We then "interpret" K as the "amplitude" to go from x' to x in time t,

and then we just add up over all x', the Feynman path idea. This K is called "the **free particle propagator**", and this important notion of a propagator appears on page 61 of Saxon.

4. Free particle packet in momentum space: the E operator. The solution here is much simpler: $\varphi(p,t) = \varphi(p,0)\, e^{-iHt}$ but he does not use H. So even with no SE yet, we know this fact for our packet! More stuff that just falls out of Fourier. By looking at the <E> in p-space, we find that $E = +i\hbar\, \partial_t$ and we are inching ever closer to the SE. Of course from $p^\mu = +i\hbar\partial^\mu$, we are not too surprised at this result.

5. Gaussian packet moving in time. We already got the propagator K in Appendix I, so if we now jam in a Gaussian for $\psi(x,0)$ we can compute $\psi(x,t)$. Again, this is done in Appendix I and the result is then displayed in (21) [the student notices that equations are getting larger as we move forward in the book] The result has the properties Saxon has already demonstrated in general, it moves at $v_g = v$, and spreads. If you set $\hbar$=0, the spread stops and you are classical. If you set the width L = 0, you get $\rho(x,t)$ = a delta function trajectory, again classical: <u>in this limit, a QM point particle goes in a classical trajectory</u>, which here is a straight line since a free particle. Chances of being off this line are 0. Very good.

6. The Free Particle SE (66). Saxon has deferred this for 66 pages of his 400 page book, perhaps a novel feature of his book. Since we have an integral expression for $\psi(x,t)$ we can show by doing the time and then the double space derivative that it satisfies the SE. But of course the plane wave does and everything is made of plane waves, so reader should not be too shocked. We can think of $H = p^2/2m$ as an "operator equation" indep of rep if we want. The FP SE is very simple in p-space of course, $\varphi(p,t) = e^{-iEt}\varphi(p,0)$

7. Probability conservation. Claim that were SE not linear in t, would not get prop conservation. Recall that this is the issue with the K-G equation before the negative energy solutions were understood. Second point is that complex numbers are significant in QM, and if you get rid of them, fine, but you have to represent a state by a 2-component vector, see p 71.

8. Dirac Bracket Notation (72)

9. Stationary States. We separate the t and x variables and find that $\psi_E(x)$ solves the **TISE** and this is called a stationary state since it has no time in it. Still no potential V yet in this book!

10. Particle in a Box. No mention of V, just that $\psi = 0$ at the walls. This is the first eigenvalue problem, and we get sine type solutions and $E \sim n^2$ where n is the quantum number. Saxon then considers a packet in this box with coefficients A_n. Usual results here until we get to (43) where he has exposed what must be the propagator K for this problem. It has the characteristic form of $K(x',x't) = \Sigma_n \varphi_n^*(x')\, \varphi_n(x) e^{-iEnt/\hbar}$ which we see many times in later QM readings. This shows that at t=0 have $\delta(x'-x)$. This general result would be true for any problem with any potential, and here we just happen to have V = 0 and φ_n = simple sines. For this problem he writes out the propagator sum in (45). I remember being a bit amazed by this. He says the packet bounces without spreading which I don't think is quite true because we know that a free packet will spread. But if box is small, maybe it undoes its spread with each bounce.

11. Summary. Not bad.

Chapter V. Schrodinger's Equation (84)

I think we are now going to repeat a lot of things covered above, the usual teaching method.

1. Probability conservation. If assume that $H\psi = E\psi$ without knowing what H is, we can still prove that H is Hermitian. This is done in x-space.

2. Hermitian operators. Operator is A, and $\langle A\varphi|\psi\rangle = \langle\varphi|A\psi\rangle$ is what Hermitian means in Dirac. Defines $A^\dagger$ and does all the usual stuff.

3. Correspondence Principle. Looks at time derivatives of expectation values of operators in an **Ehrenfest** type manner. This shows that H satisfies Hamilton's equations in the classical limit and H must therefore be the **Hamiltonian**, and so this long word appears for the first time in the book on page 94. For the first time, V(x) appears on page 94 which we add to $p^2/2m$ to get H.

4. The SE in x-space and in p-space. All familiar to me, section ends with a comment that usually QM is developed in a different manner where the SE appears right at the start. Well just pedagogy really, once you know the answer. In any event, we have now arrived and are ready to do problems.

5. Stationary states. All familiar, comment on GSO for degenerate states. Adds the closure/completeness condition for a set of eigenstates. No mention of "matrix mechanics" yet in the book, but of course I am constantly reminded of the matrix version of GSO.

6. Eigenfunctions and eigenvalues of Hermitian Operators. (101) Operator A, eigenvalue a.

7. Simultaneous Observables and Complete Sets of Operators. If A and B are operators for simultaneous observables, then [A,B] = 0. Talks about ψ_{ab} which is simul an eigenstate of both operators and likes using the word "complete" here. Think H atom: operators L_z and L^2 and H commute and their simultaneous eigenfunctions $\psi_{E\ell m}$ form a complete set, that is his point.

8. The Uncertainty Principle. This is now stated and then proved for two arbitrary operators A and B. The RHS is 0 if the operators commute. A condition (50) is given for achieving the minimum uncertainty. Then we look at the example of A = p and B = x. Then using (50), he shows that the Gaussian is the minimum uncertainty packet.

9. Wave packets and their motion. Restatement of the usual form of the propagator K in terms of the eigenfunctions, now we have V present I guess.

10. Summary: the Postulates of QM (111). This is a very well stated compact list of items. He probably thought hard about how to write this list. All very familiar to me.

Chapter VI. States of a Particle in 1D (116)

1. General Features (116). This is a very good section which I probably buzzed over in 1969. For the arbitrary potential shown, four regions are identified. High energy gives waves going in both ways with no restrictions so "double degenerate, continuous spectrum". Lower down you bounce off the right side and the requirement of expo decay there says still continuous spectrum, but only one solution, non-degenerate. Lower down still we have two turning points, so need expo on both sides, no degeneracy AND only discrete energies will work.

2. Parity Operator. P has eigenvalues ± 1, can decompose any function into sum of eigenparity functions. For a symmetric potential, [P,H] = 0 so it provides a good quantum number, though this is not quite how Saxon says it.

3. The Square Well (121). This is our first real QM problem of interest, and we solve it for the two parities separately. Sadly, we are stuck with the transcendental equation for the eigenenergies, but we get a nice general picture as shown on page 126. We get sine and cosine functions inside (for our two parities) and BC's match to expo taper on the two sides.

4. The Harmonic Oscillator (126). Right off the bat we go for a Frobenius solution, that name not used. But first a change of variable to dimensionless y from x, and then a functional change of form to u(y) pulling out an exponential factor based on looking at the expected large-x solution of the SE. Truncation of the u(y) power series leads to $(n+1)\hbar\omega$ eigenenergies, but they alternate in the two parity families. The lowest polynomials are stated, then we are told they are Hermites. We are not sent off to a special functions book, it is all done right here.

At this point, we are sent off in the direction of the creation operator representation using operators a and $a^\dagger$ defined as certain linear combinations of the operators x and p. Then $H = \hbar\omega\,(a^\dagger a + 1/2)$. He shows that these are raising and lowering operators when they act on eigenstates, hence the name creation and annihilation. Hence, you can write $\psi_n = (a^\dagger)^2\psi_o$ with suitable normalization factors as in (47). This leads to the interesting Rodriguez-like formula for the Hermites in (49). To the young reader, this must seem like so much jibberish, s/he knowing not that QFT is based on this idea.

5. The Creation Operator Representation (138). We already know that a and $a^\dagger$ are lincom x and p, so things like (54) seem obvious. By plugging away, Saxon eventually gets to the generating function expression for the Hermites in (63) and the corresponding Rodriguez finally appears. I have the feeling this whole section was sort of inserted into the book at a later time. An obvious place to insert it is right after the HO discussion. I think it makes calculations of the next section easier, however, and maybe that is the "why", as well as the field theory connection. A result of this section he will use is (61) which gives the solutions ψ_n as a Mellin-Barnes type integral over $da^\dagger$ where the integrand is just a power times a simple exponential, all of which looks very weird. Reader does not like seeing $a^\dagger$ used as an integration variable, but it avoids having another symbol like b. So this integral representation is just that of a power times a shifted gaussian.

6. Packet in the HO potential (144). We first review our general packet knowledge, then we insert the HO eigenfunctions into the usual sum which represents the propagator K. We end up with a double-Mellin of an exponential of another generalized gaussian, and the result is just quoted in (68), which looks pretty messy indeed. Various properties of this K are then found on page 145. We see that something periodic is happening. If we then assume a starting spatial Gaussian of width L and speed p_0/m, we can insert this K thing into our integral rep and compute $\psi(x,t)$ and then $|\psi|^2$ is a delightfully simple result

(73) which shows that the packet probability has a center point x(t) that does what a harmonic oscillator is supposed to do. The width oscillates in sync, being maximal in the center position. If you choose just the right gaussian width L, then the width never changes during oscillation. Again, I think the creation stuff was needed to make the computations required here all be simple Gaussian integrals.

7. Continuum States in a Square Well (147). OK, so much for bound states, we are on to scattering theory now! We have moved from Schiff Chapter 4 to Schiff Chapter 5, but still all just 1D. We are 37% through the book at this point. So for the square well we have the 3 regions, do all the BC's, all the very ugly math is shown in detail and we end up with the R and T coefficients. For the "well" we get the transmission resonances. The equations are repeated for the "post" and we get the tunneling effect.

8. Continuum states in general: probability flux. This is given by the usual expression here as (95) 1D. For the square well problem just done, we find that flux ~ T on the right, and ~(1-R) on the left.

9. Wave packet passing through a potential. I am not sure what the point is here. Yes, we can make a packet and we can watch it move. In (97) we have sort of $e^{ikz} + \rho e^{-ikz}$ for each energy component, then we sum over k (E) with some weight f(E). Then g(E) is f but centered on the mean energy E_o I guess. Then η is the energy offset from E_o. And then h(x) is the original packet envelope. The packet then seems to move linearly. Then the transmission amplitude is τ and is written as |T| times a phase shift $\delta(E)$, and we find that the packet will have a DELAY that is $\hbar\, d\delta(E)/dE$ as in (101). So he is making a point that if you knew the phase of τ, you could compute this delay. And there is also spreading. I think this section is just meant as a qualitative discussion of 1D scattering. His main result I think is (100) which says that at $x\rightarrow\infty$, your original packet -- which might have been a mess when it was at small x -- recovers itself and still has that shape h(x), but picks up a delay and some distortion. This would be the thing I would want to show, seeing that it works so nicely that way in the numeric work. You might think that a potential might completely smash an incoming packet into smithereens. He has not really given an intuitive reason why this does not happen, just a complicated math presentation.

10. Numeric Solution for Packet (158) Here we get the same 1D stuff as shown in Schiff, and the reconstitution of the packet is called "rather remarkable", but my intuitive explanation is not found. This work was just completed in time for We see that temporary bound state in the well case due to a resonance there. I think my Schiff notes probably are useful in this area. He concludes with comments on doing numeric work, giving the simple stupid method then saying that Runge-Kutte and other methods are much better. I have all these things under my belt from reading Scheid, but would have to review those notes to get the information restored.

Chapter VII. Approximation Methods (174)

1. The WKB Approximation

I have just finished reading Schiff's version of this subject and want to now see what Saxon has to say. His approach is different. He assumes the form (2) with two unknown functions A(x) and S(x). By writing out the exact SE and ignoring certain terms for small $\hbar$, he arrives at "the usual" solution for S(x) as shown in (4), being the integral of p(x), ie, being the abbreviated action. But then he finds that A(x) = $k^{-1/2}$ as in Schiff, but interprets this as required to maintain probability conservation, good. So we get the

Saxon version of the WKB wavefunction in (6), where he uses x_0 instead of x = 0. My pencil markings show that I read this section very carefully in Hillis library many years ago! He then works on the conditions of validity and I think does this better than Schiff does, but gets the same basic results on page 177. He then goes a step beyond Schiff and obtains the first correction term beyond the WKB formula and this is shown as the ΔS contribution in page 178 equation A. He regards then (10) as the exact WKB approximation condition of validity, but it is a complicated integral of k(x). On page 179 he then provides a simplified version of this condition in (8a). This involves $k'(x)_{max}$, k_{min} and q which is the number of sign changes of a certain function of k(x) in the interval of interest. On page 180, he is ready to move into some examples.

Notice that there are no Bessel J functions mentioned at all by Saxon, as I suspected would be the case. Also, in Schiff the WKB appears in the "bound state approximations" chapter, but Saxon is going to open with a scattering application. [Saxon does mention the Bessel J in his page 182 footnote.]

Example #1. This is a 1D scattering problem where a plane wave starts at the far left and scatters off some kind of localized potential that varies smoothly and our E always lies above V(x). Classically if we putt a golf ball on this little mini golf range, there will be no reflection, and that is also the case in WKB, as we see below, showing again its classical flavor. However, there will be some slowing down of the ball as it goes over some little potential hump (or a speeding up if it is a valley). To handle this example, he starts with the WKB form page 180 A. Notice the useful appearance of $\psi(x_0)$ in this expression, which makes things sort of propagator like -- a good way to normalize things. At $x_0 = -\infty$ we install our plane wave and some computation then gives us page 181A for the result. We can then take the limit $x \rightarrow +\infty$ and we get B which shows that the transmission amplitude is unity, so no reflection as predicted. But there is a phase and we can relate the derivative δ(phase)/δE to the time delay, and we obtain the exact result for this time delay you would get computing this classically. So this example shows the classicality of the WKB approximation.

Example #2. This is a generic consideration of the bound state problem with some smooth potential. Our WKB form, recall, looks like $\exp(\pm i\xi)/\sqrt{k}$ and these are the two solutions we can play with. Obviously you could think of this as sine and cosine, or $\sin(\xi + \delta)$ as Saxon writes in (11). At this point Saxon makes his great comment that, when the dust settles on the Bessel function stuff (footnote page 182), the right solution is this sine form but you extend it beyond the turning point on each side by 1/8th wavelength, which is $2\pi/8 = \pi/4$ of phase on each side. Maybe this is the hint I need to clear up some Schiff problems I have. // Yes it was, and I discuss this thing in my Schiff Chapter 8 meta notes.

So just as Schiff did, Saxon comes up with the modified Bohr-Sommerfeld rule which can then be used to compute eigenenergies E. Of course he does this with the arm-waving 1/8th wave rule. Still, I like it a lot.

Example #3. If you apply the above method to the famous harmonic oscillator problem in 1D, the Bohr Sommerfeld gives *exactly* the right eigenenergies even for a small number of waves where you are far from the WKB validity region, ie, far from classical. This is regarded as a quirk, but of course there is some underlying reason (like O(4) or SU(3)). You don't get perfect HO wavefunctions near n=0 of course.

2. Rayleigh-Ritz variational method (184)

In his opening discussion, Saxon points out that the ratio (15) is stable against variation in the usual Goldstein sense. If you vary the functions ψ and ψ^* separately, you find that there is no linear term in the parameters if you write $E' = f(\alpha,\beta)$. The Schrodinger Equation is the Euler Equation of this variation! So he is sort of stating a variational form of QM which I have not really seen elsewhere for QM. So he concludes that E' is quadratic or higher in the parameters. This is an interesting formulation of QM: the correct ψ is the one that makes $\delta E' = 0$.

But when we come to using this idea, Saxon reverts to the normal Schiff discussion. For the ground state, we get the inequality shown bottom of page 186. He then has a lot of discussion about how you need to select an intelligent trial function for your variational approach. He does show explicitly that if your trial function is orthogonal to all lower states (which is generally not easy to arrange), then you can get a simple inequality for a higher level. The higher you go, the harder it gets, so he says this method works best for low-lying states and thus serves as a complement to the WKB that works best for classical high states. In a symmetric potential, ground state is even, so you should use an odd trial function and then you can get an upper bound for the first excited state.

He then does one simple example. He considers the HO with a trial function being a quadratic hump as in (19). The width is 2a and a will be the variation parameter. He does the integrals, and finds the interesting ground state result $E' = \hbar\omega/2 * \sqrt{12/11}$ which is larger than the correct answer by 5%, not bad. More examples are embedded in his problems.

3. Stationary State Perturbation Theory (Non-Degenerate Case). (189)

[1.6.09] I am reading this now after doing my own theory, and after reading Schiff on the subject as well. Saxon starts off a little differently than Schiff and I do. He uses coefficients c_{in} which are my B_{ni} where we have the summation index in a different position. Both Saxon and I have these symbols which are summed to all orders. There are no power series yet. Saxon then inserts his expansion of the fully corrected wavefunction into the full SE and he gets page 191 (26) which is a matrix equation for the coefficient matrix c_{in}. Notice that this is really M^2 equations since you can set n and j to 1..M, where I will assume M is the size of our problem's Hilbert Space. He thinks of $N = \infty$ as it is for such problems as the 1D HO or particle in a box, etc. Really, he has just restated the full problem in matrix form.

I am completely happy with all equations on **page 191**, they get red checks. We are still doing all orders at once. And I agree that the correction c_{jn}/c_{nn} is order λ and higher, and of course goes to zero as $\lambda \rightarrow 0$. What Saxon does on page 191 is set up a systematic scheme of "successive approximations" as he calls it. We have λ on the RHS of all equations. Look at (28) and (29). (29) says $c_{in}/c_{nn} \sim \lambda$ and thus we can use just the first term in (29) for c_{in}/c_{nn} to this order, and the first term in (28) for the energy. We then take our first order coefficients c_{in}/c_{nn} and plug them on the right side of both equations and we then get a second order term for each, and it seems very reasonable that in this manner you can quickly build up a power series for energy and for coefficients. I like it.

I am now happy as well with **page 192** and he shows the solutions through second order at the bottom, very nice. We don't have any "general power series" equations, we are just building up one level at a time.

Comment: Look at (35) on the bottom of p 192. It shows both the ε_1 and ε_2 corrections to the energy, so he got this pretty fast. In my full degenerate notes I arrive at the ε_2 as follows: (for me, state mi is one of the degenerate states with energy E_m and labeled by i)

$W_{mi,2} = \langle u_{mi}| H' | \psi_{mi,1}\rangle$

$= \langle u_{mi}| H' | [\{ \Sigma_{j\neq i} B'_{ij,1} |u_{mj}\rangle \} \oplus \Sigma_{k\neq m} B'_{ik,1} |u_k\rangle]$

$= \Sigma_{k\neq m} B'_{ik,1} \langle u_{mi}| H' |u_k\rangle$ // other states in the m subspace do nothing

$= \Sigma_{k\neq m} \langle u_{mi}| H' |u_k\rangle \langle u_k| H' |u_{mi}\rangle / (E_m - E_k) = \Sigma_{k\neq m} |H'_{k,mi}|^2 / (E_m - E_k)$

since

$B'_{ik,1} = \langle u_k| H' |u_{mi}\rangle / (E_m - E_k)$

So Saxon just gets to the energy formula by a different path, but it is the same formula.

Page 193 makes some excellent comments not found in Schiff at all.

• Nobody does perturbation theory beyond second order, and only does that if necessary.

• Think of H'_{ij} as a measure of **"distorting forces"** in the problem. In the first order correction, we don't account for wavefunctions adjustment to these forces. If the forces are "attractive", our energy is lowered by the first order correction, otherwise are raised. Could have either sign. In the second order we are allowing the wavefunctions to adjust a bit to these distorting forces, and we expect this to lower energy, so we expect the last term in (35) to be negative. This means that denominators "tend to be negative" on average (our expectation). For n = a ground state, all other states lie above, all denominators *are* negative, and our expectation is proven. For higher than ground state, we don't have a proof. Saxon compares this to polarization distortion or strain distortion. So at this point, we are 1/3 down page 194.

Page 194: Suppose H_0 is even under parity. We know that that solutions u_k can then be classified as even or odd. For the H atom, for example, $H_0 = p^2/2m + k/r$ is certainly even. Now, suppose H' is odd under parity. Then consider the diagonal matrix elements of H'. We have $\langle u_k|H'|u_k\rangle = 0$ regardless of whether we pick u_k to be even or odd!

His footnote gives one example which is Stark Effect. In a 1D problem, know that H' = eV where **E** = $-\nabla$V so constant E means linear V through the origin which is an odd function. I guess in 3D, if you pick the z direction, V is odd in that direction so again H' is odd in that sense, we shall see later. The point is that in Stark Effect, there is no first order energy correction due to this selection rule! In time dependent perturbation theory, we shall see similar selection rules based on parity. One might expect other symmetries to create similar selection rules.

Page 195: I skip the details here, his subject is the convergence of the perturbation series. Starting with the true (38) he ends up with (39) which is a condition that "must be true", where $\Delta\varepsilon_n$ is to nearest neighbor of a state n. I think he is just saying that if (39) is not true, then your perturbation theory is not going to converge. Right now, this subject is not of great interest since I am mainly eager to see how Saxon handles the degenerate situation. Earlier Saxon gave $\lambda H'_{ni} << (E_n - E_i)$ as a *necessary* condition for convergence, but even if true, you might still diverge. This is always an interesting topic with series, but again, I am a big "don't care" right now.

Page 196: Saxon's first example is to add an H' Gaussian potential to the usual quadratic 1D HO potential, with parameter α as shown and size V. He computes the first order correction to the ground state but does not show the computation. We would just do the integral of the ground state expo squared times H' as shown, and it is some kind of simple Gaussian integral. He then asks about convergence in this toy problem. He says the second order calculations are messy, so he will use his little rule (39) of page 195 to estimate a rule for convergence that puts a condition on parameters α and V. Again, right now these are details out of the main flow that I will not study right now.

Page 197,198: This time he adds an x^4 correction to the 1D HO potential with parameter b. This is the anharmonic oscillator and is a more practical problem for the real world. He is of course then faced with computing $\langle n|x^4|n\rangle$ for the HO states $|n\rangle$. I just did this in detail for then $\langle n|x^2|n\rangle$ situation in Schiff's HO example, and of course in my situation it was terms like $aa^\dagger$ that contributed, and here it will be terms like $aa^\dagger aa^\dagger$. You must raise and lower an equal number of times as you apply to the right so you have something left over to get a non-vanishing scalar product closure. It turns out that the sum of all these terms is not too bad, and he states it on page 198 where I wrote "good" a long time ago in pencil. Then (41) is our conclusion for the first order energy correction. If you write this as in (42), you see that the energy transition gaps which the spectroscopist measures will detect the n^2 term only. I think the vibrational situations encountered in chemistry have exactly such anharmonicity. Saxon claims that that if you have an x^3 anharmonic term, you get the same type result, so these two terms get messed together. Of course the x^3 term has the problems of the next little discussion -- metastable states.

Page 199-201. What happens if you have a *negative* quartic term for H' in the 1D HO example? The potential is then as shown in the page 200 picture. If you create a nice packet that sits inside for a while, you can regard it as a meta-stable bound state, and you can use perturbation theory on such a state as if it were a real bound state. A real bound state has no energy spread, but a meta-stable state does have an energy spread which is then inversely proportional to its lifetime τ as on page 201. I could see how this might be a practical problem in some situation.

Comments: This was a typically excellent Saxon book section, quite long at 12 pages (see all my notes above!). There was no dishonesty, all was clear, and he dug deeper on convergence that he had to. His book is 1968 and Schiff's 1955 (later edition 1968) probably already had the x^2 HO perturbation example, so Saxon chose different examples, to his credit.

4. Matrices. This seems an odd place to inject this subject. The indices on the matrices here are eigenstate labels, and I think he is thinking discrete labels. If your eigenstates n are those of A, then matrix A will be diagonal in that basis. But there is nothing said about "matrix mechanics" or any reference to history here.

OK, the reason this section is here is that in 1968, students were "weak" on the matrix subject and linear algebra in general, and Saxon is pumping the student up a little because matrices are going to be heavily involved in the next section on degenerate perturbation theory which has caused me (in Schiff) so much trouble.

5. Degenerate or Close-Lying States (p 204)

Comment:

[1.6.09] Saxon has brought up a *third* problem, one which I had not thought about, namely, a set of N states which are very closely spaced (but not necessarily degenerate) relative to the validity rule $\lambda H'_{jk} << E_k - E_j$. In this section he talks about the situation with N = 2, which he indicates with labels n and ℓ, but I prefer using 1 and 2. In his math, he works "to all orders", not making explicit power series as Schiff does. He maintains in his math the distinction between what I would then call E_{m1} and E_{m2} but which he calls ε_n and ε_ℓ . In my verifications below, I assumed exact degeneracy because that was the problem I cared about when I was reading this on 1/6/08.

Saxon's approach is *very different* from Schiff's, amazingly much so.

- There are no explicit power series expansions, but we are given a successive approximations rule.
- He does not normalize ψ in the special way that makes $\langle u_{mi} | \psi_{mi} - u_{mi} \rangle = 0$.
- He does not "require" that H' must start off being diagonal in the u_{mi}, though he does end up with a result I talk about below that gives the required linear combinations.

Having done all of the below, I must say I am not all that thrilled with Saxon's approach either (that is, I don't like Saxon *or* Schiff). I am looking for something more systematic that handles N degenerate states and tells me exactly how to compute things through say third order, or perhaps all orders. I am convinced that in such a systematic solution, you really should diagonalize H' as your very first step, but neither Schiff nor Saxon mentions this.

Notes on the text

We start by rewriting the exact equations A on page 191 by breaking out the state ℓ from the sums so that the n and ℓ terms are treated on an equal footing since this pair is now assumed degenerate or at least very close. In all my stuff below, I assume fully degenerate. The pair of equations 191 A is now replaced with the three equations page 205 (51) which I agree with.

Why do I agree? Take the first equation in page 191 A and first move the H'_{nn} term to the LHS. Then extract the RHS term with $i = \ell$ and move it also to the LHS. So this verifies the first of (51).

Now getting the second of (51) is harder. I had to go back to page 191 and pencil things in at the bottom. You start with (26) which is rewritten as A1, then replace n with ℓ only where I have marked with little vertical segments, and this gives the pencil result at page bottom there.

He then claims this: the third equation of (51) says c_{jn} is order λ ($j \neq n$ or ℓ) and therefore the RHS's of the first two equations are order λ^2 and therefore we can dump these RHS's in order to do an order λ computation as shown in page 205 equations A.

Before taking another step, I want to connect this with what I have done in my Schiff-related notes. Saxon's results do not quite look familiar to me. Let me try to start off as Saxon does, but in my own notation. Saxon does not do the fancy renormalization that Schiff does, so use non-primed B coefficients:

$$\psi_{mi} = \{ u_{mi} + \Sigma_j B_{ij} u_{mj} + \Sigma_{k \neq m} B_{ik} u_k \}$$

Moreover, Saxon is going to include the lone u_{mi} in the first sum. So let me define some new coefficients like this so I can match Saxon:

$$D_{ik} = B_{ik}$$
$$D_{ij} = B_{ij} \qquad i \neq j$$
$$D_{ii} = 1 + B_{ii} \qquad i = j$$

so I then have

$$\psi_{mi} = \{ \Sigma_j \; D_{ij} \; u_{mj} + \; \Sigma_{k \neq m} \, D_{ik} \, u_k \}$$

If I put this into the SE which is $H\psi_{mi} = W_{mi}\psi_{mi}$ I get this

$$(H_o + \lambda H') \{ \Sigma_j D_{ij} \; u_{mj} + \; \Sigma_{k \neq m} \, D_{ik} \, u_k \} = W_{mi} \{ \Sigma_j D_{ij} \; u_{mj} + \; \Sigma_{k \neq m} \, D_{ik} \, u_k \}$$

where I am now doing things to all orders at once, no series stuff. Now get the λH' stuff isolated on the RHS:

$$(W_{mi} - H_0) \{ \Sigma_j D_{ij} \; u_{mj} + \; \Sigma_{k \neq m} \, D_{ik} \, u_k \} = \lambda H' \{ \Sigma_j D_{ij} \; u_{mj} + \; \Sigma_{k \neq m} \, D_{ik} \, u_k \}$$

$$\Sigma_j D_{ij} \; (W_{mi} - E_m) u_{mj} + \; \Sigma_{k \neq m} \, D_{ik} \, (W_{mi} - E_k) u_k = \{ \Sigma_j D_{ij} \; \lambda H' u_{mj} + \; \Sigma_{k \neq m} \, D_{ik} \, \lambda H' u_k \}$$

$$(W_{mi} - E_m) \, \Sigma_j D_{ij} \, |u_{mj}\rangle + \; \Sigma_{k \neq m} \, D_{ik} \, (W_{mi} - E_k) \, |u_k\rangle = \{ \Sigma_j D_{ij} \; \lambda | \, H' \, |u_{mj}\rangle + \; \Sigma_{k \neq m} \, D_{ik} \, \lambda | \, H' \, |u_k\rangle \}$$

This is not a path I followed before, it's a new path. So we have the two kinds of closure to do:

A. Close with $\langle u_{k'}|$:

$$\Sigma_{k \neq m} \, D_{ik} \, (W_{mi} - E_k) \delta_{k,k'} = \Sigma_j D_{ij} \; \lambda \langle u_{k'}| \, H' \, |u_{mj}\rangle + \; \Sigma_{k \neq m} \, D_{ik} \, \lambda \langle u_{k'}| \, H' \, |u_k\rangle$$

$$D_{ik'} \, (W_{mi} - E_{k'}) = \Sigma_j D_{ij} \; \lambda \langle u_{k'}| \, H' \, |u_{mj}\rangle + \; \Sigma_{k \neq m} \, D_{ik} \, \lambda \langle u_{k'}| \, H' \, |u_k\rangle$$

$$D_{ik} \, (W_{mi} - E_k) = \Sigma_j D_{ij} \; \lambda \langle u_k| \, H' \, |u_{mj}\rangle + \; \Sigma_{k' \neq m} \, D_{ik'} \, \lambda \langle u_k| \, H' \, |u_{k'}\rangle \qquad k \leftrightarrow k'$$

$$D_{ik} \, (W_{mi} - E_k) = \Sigma_j D_{ij} \; \lambda H'_{k,mj} + \; \Sigma_{k' \neq m} \, D_{ik'} \, \lambda H'_{k,k'} \qquad k \leftrightarrow k'$$

This is an equation for every i in $\mathcal{H}^{(m)}$ and every k in $\mathcal{H}^{\perp}$. This is in fact **the *third* of equations (51)** on Saxon page 205. For Saxon i = 1,2 so we have

$$D_{1k} \, (W_{m1} - E_k) = D_{11} \; \lambda H'_{k,m1} + \; D_{12} \; \lambda H'_{k,m2} + \Sigma_{k' \neq m} \, D_{1k'} \, \lambda H'_{k,k'} \qquad i=1$$
$$D_{2k} \, (W_{m2} - E_k) = D_{22} \; \lambda H'_{k,m2} + \; D_{21} \; \lambda H'_{k,m1} + \Sigma_{k' \neq m} \, D_{2k'} \, \lambda \, H'_{k,k'} \qquad i=2$$

Notice that this mixes the interior and exterior D_{rs} coefficients.

B. Close with $\langle u_{ms}|$:

$$(W_{mi} - E_m)[\,\Sigma_j D_{ij} \langle u_{ms}|u_{mj}\rangle] \;+\; \Sigma_{k\neq m} D_{ik}\,(W_i - E_k)\langle u_{ms}|u_k\rangle$$

$$= \{\,\Sigma_j D_{ij}\;\lambda\langle u_{ms}|H'|u_{mj}\rangle + \;\Sigma_{k\neq m} D_{ik}\,\lambda\langle u_{ms}|H'|u_k\rangle\}$$

$$(W_{mi} - E_m)D_{is} \quad = \{\,\Sigma_j D_{ij}\;\lambda\langle u_{ms}|H'|u_{mj}\rangle + \;\Sigma_{k\neq m} D_{ik}\,\lambda\langle u_{ms}|H'|u_k\rangle\}$$

Now expose the term D_{is} in the RHS sum (ie, j=s) and move it to the LHS

$$(W_{mi} - E_m)D_{is} \;- D_{is}\lambda\langle u_{ms}|H'|u_{ms}\rangle$$

$$= \{\,\Sigma_{j\neq s} D_{ij}\;\lambda\langle u_{ms}|H'|u_{mj}\rangle + \;\Sigma_{k\neq m} D_{ik}\,\lambda\langle u_{ms}|H'|u_k\rangle\}$$

<u>First, set s = i to get:</u>

$$(W_{mi} - E_m)\,D_{ii} - D_{ii}\lambda\langle u_{mi}|H'|u_{mi}\rangle$$

$$= \{\Sigma_{j\neq i} D_{ij}\;\lambda\langle u_{mi}|H'|u_{mj}\rangle + \;\Sigma_{k\neq m} D_{ik}\,\lambda\langle u_{mi}|H'|u_k\rangle\}$$

$$(W_{mi} - E_m - \lambda\, H'_{mi,mi})\,D_{ii} \;- \Sigma_{j\neq i} D_{ij}\;\lambda\, H'_{mi,mj} \;=\; \Sigma_{k\neq m} D_{ik}\,\lambda\, H'_{mi,k} \qquad i = 1,2..N$$

This is seen to be **the *first* of equation (51)** on Saxon page 205. My state mi is his state n. He has only one partner state he calls ℓ but I have N-1 partner states in the LHS sum. I have not used "my" fact that you have to choose states that diagonalize H'. Saxon obviously is not doing that, so this issue has to be resolved at some point. My equation above applies for all states mi in $\mathcal{H}^{(m)}$. Saxon will have two of these equations then, here they are:

$$(W_{m1} - E_m - \lambda\, H'_{m1,m1})\,D_{11} \;-D_{12}\;\lambda\, H'_{m1,m2} \;=\; \Sigma_{k\neq m} D_{1k}\,\lambda\, H'_{m1,k} \qquad i = 1$$

$$(W_{m2} - E_m - \lambda\, H'_{m2,m2})\,D_{22} \;-D_{21}\;\lambda\, H'_{m2,m1} \;=\; \Sigma_{k\neq m} D_{2k}\,\lambda\, H'_{m2,k} \qquad i = 2$$

<u>Second, set s ≠ i to get:</u>

$$(W_{mi} - E_m)D_{is} \;- D_{is}\lambda\langle u_{ms}|H'|u_{ms}\rangle \;= \{\,\Sigma_{j\neq s} D_{ij}\;\lambda\langle u_{ms}|H'|u_{mj}\rangle + \;\Sigma_{k\neq m} D_{ik}\,\lambda\langle u_{ms}|H'|u_k\rangle\}$$

$$(W_{mi} - E_m \;- \lambda\langle u_{ms}|H'|u_{ms}\rangle)\,D_{is} \;= \{\,\Sigma_{j\neq s} D_{ij}\;\lambda\langle u_{ms}|H'|u_{mj}\rangle + \;\Sigma_{k\neq m} D_{ik}\,\lambda\langle u_{ms}|H'|u_k\rangle\}$$

$$(W_{mi} - E_m \;- \lambda\, H'_{ms,ms})\,D_{is} \;= \Sigma_{j\neq s} D_{ij}\;\lambda H'_{ms,mj} + \;\Sigma_{k\neq m} D_{ik}\,\lambda H'_{ms,k}$$

$$-\;\Sigma_{j\neq s} D_{ij}\;\lambda H'_{ms,mj} \;+ (W_{mi} - E_m \;- \lambda\, H'_{ms,ms})\,D_{is} \;=\; \Sigma_{k\neq m} D_{ik}\,\lambda H'_{ms,k}$$

This is seen to be **the *second* of equation (51).** For each pair i≠s, this gives two equations. Here they are for Saxon:

$$-\ D_{11}\ \lambda H'_{m2,m1}\ +(W_{m1}-E_m\ -\lambda\ H'_{m2,m2})\ D_{12}\ =\ \Sigma_{k\neq m}\ D_{1k}\ \lambda H'_{m2,k} \qquad i=1\ \ s=2$$

$$-\ D_{22}\ \lambda H'_{m1,m2}\ +(W_{m2}-E_m\ -\lambda\ H'_{m1,m1})\ D_{21}\ =\ \Sigma_{k\neq m}\ D_{2k}\ \lambda H'_{m1,k} \qquad i=2\ \ s=1$$

So I have now found the generalizations of (51), and I have written them all out for N=2. Here now I gather the specific three equations that Saxon shows for his case (three of 6 possible equations)

$$(W_{m1}-E_m-\lambda\ H'_{m1,m1})\ D_{11}\ -D_{12}\ \lambda\ H'_{m1,m2}\ =\ \Sigma_{k\neq m}\ D_{1k}\ \lambda\ H'_{m1,k} \qquad i=1$$

$$-\ D_{11}\ \lambda H'_{m2,m1}\ +(W_{m1}-E_m\ -\lambda\ H'_{m2,m2})\ D_{12}\ =\ \Sigma_{k\neq m}\ D_{1k}\ \lambda H'_{m2,k} \qquad i=1\ \ s=2$$

$$D_{1k}\ (W_{m1}-E_k)\ =D_{11}\ \lambda H'_{k,m1}+\ D_{12}\ \lambda H'_{k,m2}+\Sigma_{k'\neq m}\ D_{1k'}\ \lambda H'_{k,k'} \qquad i=1$$

To get his exact equations, you would make these substitutions:

$1 \rightarrow n$
$2 \rightarrow \ell$
$D_{rs} \rightarrow c_{sr}$ // note index swap !

I will do this explicitly just to make sure everything is kosher: (it is!)

$$(W_{mn}-E_m-\lambda\ H'_{mn,mn})\ c_{nn}\ -c_{\ell n}\ \lambda\ H'_{mn,m\ell}\ =\ \Sigma_{k\neq m}\ c_{kn}\ \lambda\ H'_{mn,k} \qquad i=1$$

$$-\ c_{nn}\ \lambda H'_{m\ell,mn}\ +(W_{mn}-E_m\ -\lambda\ H'_{m\ell,m\ell})\ c_{\ell n}\ =\ \Sigma_{k\neq m}\ c_{kn}\ \lambda H'_{m\ell,k} \qquad i=1\ \ s=2$$

$$c_{kn}\ (W_{mn}-E_k)\ =c_{nn}\ \lambda H'_{k,mn}+\ c_{\ell n}\ \lambda H'_{k,m\ell}+\Sigma_{k'\neq m}\ c_{k'n}\ \lambda H'_{k,k'} \qquad i=1$$

Of course there are other differences in notation that I leave in place. I think his presentation would have been clearer had he used just 1 and 2 so you don't confuse indices so much, so I will go back to that notation right now:

$$(W_{m1}-E_m-\lambda\ H'_{m1,m1})\ D_{11}\ -D_{12}\ \lambda\ H'_{m1,m2}\ =\ \Sigma_{k\neq m}\ D_{1k}\ \lambda\ H'_{m1,k} \qquad i=1$$

$$-\ D_{11}\ \lambda H'_{m2,m1}\ +(W_{m1}-E_m\ -\lambda\ H'_{m2,m2})\ D_{12}\ =\ \Sigma_{k\neq m}\ D_{1k}\ \lambda H'_{m2,k} \qquad i=1\ \ s=2$$

$$D_{1k}\ (W_{m1}-E_k)\ =D_{11}\ \lambda H'_{k,m1}+\ D_{12}\ \lambda H'_{k,m2}+\Sigma_{k'\neq m}\ D_{1k'}\ \lambda H'_{k,k'} \qquad i=1$$

Now here is why he picked these three of the six possible equations. (1) the first two involve D_{11} and D_{12} *only* (on the LHS). (2) The last one involves the D_{ik} which appears on the right of the first two. (3) both of the first equations contain the same variable W_{m1} (not W_{m2} for example).

So his next step is to say that the third equation shows $D_{1k} \sim \lambda$. The factor $(W_{m1} - E_k)$ is of order 1 since k is far away, so his argument is valid. Plus we know anyway that D_{ik} in general are order λ or higher.

But his argument is good, and therefore the RHS of the first two are order λ^2 or higher. THIS then leads to the little pair of equations as follows: (this is **Saxon p 205 A**)

$$(W_{m1} - E_m - \lambda H'_{m1,m1})\, D_{11} - D_{12}\, \lambda H'_{m1,m2} = 0$$

$$- D_{11}\, \lambda H'_{m2,m1} + (W_{m1} - E_m - \lambda H'_{m2,m2})\, D_{12} = 0$$

I can write this in matrix notation as follows:

$$\begin{pmatrix} H'_{11} & H'_{12} \\ H'_{21} & H'_{22} \end{pmatrix} \begin{pmatrix} D_{11} \\ D_{12} \end{pmatrix} = [\,(W_{m1} - E_m)/\lambda] \begin{pmatrix} D_{11} \\ D_{12} \end{pmatrix}$$

which is indeed an eigenvalue problem. Call the column vector (D_1). Then we have

$$H'\,(D_1) = [(W_{m1} - E_m)/\lambda]\,(D_1)$$

The secular equation is then

$$\det(\, H' - (W_{m1} - E_m)/\lambda * 1] = 0$$

which I can write out as

$$\{\, H'_{11} - (W_{m1} - E_m)/\lambda \,\}\{\, H'_{22} - (W_{m1} - E_m)/\lambda \,\} - H'_{12}H'_{21} = 0$$

$$\{\, \lambda H'_{11} - (W_{m1} - E_m) \,\}\{\, \lambda H'_{22} - (W_{m1} - E_m) \,\} - \lambda^2\, H'_{12}H'_{21} = 0$$

$$\{\, \lambda H'_{11} - W_{m1} + E_m) \,\}\{\, \lambda H'_{22} - W_{m1} + E_m) \,\} - \lambda^2\, H'_{12}H'_{21} = 0$$

$$\{\, -\lambda H'_{11} + W_{m1} - E_m) \,\}\{\, -\lambda H'_{22} + W_{m1} - E_m) \,\} - \lambda^2\, H'_{12}H'_{21} = 0$$

$$\{\, W_{m1} - E_m - \lambda H'_{11}) \,\}\{\, W_{m1} - E_m - \lambda H'_{22}) \,\} - \lambda^2\, H'_{12}H'_{21} = 0$$

and this is **Saxon equation p 205 B**. This is a quadratic, so rewrite as

$$(W_{m1} - E_m)^2 + \lambda^2\, H'_{11}\, H'_{22} - \lambda\, (W_{m1} - E_m)(\, H'_{11} + H'_{22}) - \lambda^2\, H'_{12}H'_{21} = 0$$

$$(W_{m1} - E_m)^2 - \lambda\, (\, H'_{11} + H'_{22})\, (W_{m1} - E_m) + \lambda^2\, \det H' = 0$$

The solutions here are then

$$W_{m1} - E_m = \{\, \lambda\, (\, H'_{11} + H'_{22}) \pm [\lambda^2\, (\, H'_{11} + H'_{22})^2 - 4\, \lambda^2\, \det H' \,]^{1/2} \,\}/2$$

$$W_{m1} - E_m = \{\, \lambda\, (\, H'_{11} + H'_{22}) \pm \lambda\, [(\, H'_{11} + H'_{22})^2 - 4(H'_{11}\, H'_{22} - H'_{12}H'_{21} \,]^{1/2} \,\}/2$$

$$W_{m1} - E_m = \{\, \lambda\, (\, H'_{11} + H'_{22}) \pm \lambda\, [(\, H'_{11} - H'_{22})^2 + 4\, H'_{12}H'_{21} \,]^{1/2} \,\}/2$$

and this is the result he shows in (53) but I have assumed exact degeneracy and he has allowed the two degenerate states to be "very close".

Question: If W_{m1} is supposed to be the eigenenergy of one of my two solutions, how can it have two values given by the ± here!

Answer: I think there is another eigenvalue equation we would get from the other triplet of equations that Saxon did not write, and I am guessing it would be this:

$$\begin{pmatrix} H'_{11} & H'_{12} \\ H'_{21} & H'_{22} \end{pmatrix} \begin{pmatrix} D_{21} \\ D_{22} \end{pmatrix} = [\,(W_{m2} - E_m)/\lambda] \begin{pmatrix} D_{21} \\ D_{22} \end{pmatrix}$$

and this eigenvalue equation has the SAME eigenvalues as the previous one. So we should assign one sign to W_{m1} and the other to W_{m2}.

When we solve, we get not only the eigenvalues, but the eigenvectors. Going back to our first EV equation, we had

$$W_{m1} - E_m = \{\, \lambda\,(H'_{11} + H'_{22}) + \lambda\,[(H'_{11} - H'_{22})^2 + 4\,H'_{12}H'_{21}\,]^{1/2}\,\}/2 \qquad \text{// pick + sign}$$

$$= \lambda\{\,(H'_{11} + H'_{22}) + [(H'_{11} - H'_{22})^2 + 4\,H'_{12}H'_{21}\,]^{1/2}\,\}/2$$

$$(W_{m1} - E_m - \lambda\,H'_{m1,m1})\,D_{11} - D_{12}\,\lambda\,H'_{m1,m2} = 0$$

$$(W_{m1} - E_m - \lambda\,H'_{m1,m1}) = D_{12}/D_{11} * \lambda\,H'_{m1,m2}$$

$$D_{12}/D_{11} = (W_{m1} - E_m - \lambda\,H'_{m1,m1})/\,[\lambda\,H'_{m1,m2}] \qquad \text{// second form in (54) take + sign}$$

If I have my second EV equation correct above, then all I do is change the first index on the D's and use the other energy W_{m2} and all else stays the same, so I think we should get

$$D_{22}/D_{21} = (W_{m2} - E_m - \lambda\,H'_{m1,m1})/\,[\lambda\,H'_{m1,m2}] \qquad \text{// second form in (54) take + sign}$$

where I am now saying

W_{m1} = the + sign
W_{m2} = the - sign

So this then is my justification of (54) as two separate equations in the ± sense. Now let's insert the eigenenergies

$$D_{12}/D_{11} = (W_{m1} - E_m - \lambda\,H'_{m1,m1})/\,[\lambda\,H'_{m1,m2}]$$

$$= \lambda\{\,(H'_{11} + H'_{22}) + [(H'_{11} - H'_{22})^2 + 4\,H'_{12}H'_{21}\,]^{1/2}\,\}/[2\lambda\,H'_{m1,m2}]$$

$$= \{ (H'_{11} + H'_{22}) + [(H'_{11} - H'_{22})^2 + 4 H'_{12}H'_{21}]^{1/2} \}/[2 H'_{m1,m2}]$$

where I have chosen to use the second expression in (54) whereas he uses the first. It is clear in either case that the λ cancels, as Saxon says on page 207.

Now I need to go back to my original expansion

$$\psi_{mi} = \{ \Sigma_j \; D_{ij} \; u_{mj} + \Sigma_{k\neq m} D_{ik} \, u_k \}$$

$$\psi_{m1} = \{ \Sigma_j \; D_{1j} \; u_{mj} + \Sigma_{k\neq m} D_{1k} \, u_k \} = D_{11} \, u_{m1} + D_{12} \, u_{m2} + \Sigma_{k\neq m} D_{1k} \, u_k$$

Now in this notation we know that D_{11} is large, so lets write this as

$$\psi_{m1} = D_{11} \, (u_{m1} + (D_{12}/D_{11}) \, u_{m2} + \Sigma_{k\neq m} (D_{1k}/D_{11}) \, u_k$$

Now, as we take $\lambda \rightarrow 0$, $D_{1k} \rightarrow 0$, and $D_{11} \rightarrow 1$, but the ratio (D_{12}/D_{11}) stays constant and given by the above. So in this limit we have

$$\psi_{m1} \rightarrow u_{m1} + (D_{12}/D_{11}) \, u_{m2} \qquad \text{as } \lambda \rightarrow 0$$
$$\psi_{m2} \rightarrow u_{m1} + (D_{22}/D_{21}) \, u_{m2} \qquad \text{as } \lambda \rightarrow 0$$

and this, as Saxon says, tells us the right linear combinations we should have started with. Very strange how this comes out in the end like this.

He concludes this section with two short "special examples".

Comments added later 3/6/09. Saxon allows the two degenerate states to be "very close" so we have then that $\mathcal{E}_\ell \neq \mathcal{E}_n$ and you then get (53) which gives the eigenenergies from the level 1 secular equation. He then defines $\overline{E}$ as the average of the two state energies corrected only through first order, and he defines $\Delta\overline{E}$ as the difference of these same two things. He can then rewrite (53) as in page 206 A. The graph on page 207 then shows these two thru-second-order-corrected energies as a function of the first-order difference which is ~ Δ. If the two states are exactly degenerate (through first order), the $E_n^{\pm}$ are the two values at the center of the graph, and the second order shifts are $\pm\lambda \, |H'_{\ell n}|/\overline{E}$ from p 206 A. If your two states are NOT degenerate through first order, then there is some $\Delta > 0$, say, and then the two state energies (through second order) $E_n^{\pm}$ are in fact farther apart! Somehow having more separation through first order causes more separation through second order. If you were to set $\lambda^2 = 0$ in p 206 A, you would be throwing out the second order (by itself) correction and then $E_n^{\pm} = 1 \pm \Delta/2$ and these are the dotted lines in the picture. So the second order correction by itself is the distance between the curves and the dotted lines, and this second order correction by itself is maximal when the two states are degenerate through first order. There is this idea that for a pair of degenerate (through first order, Δ=0) or nearly degenerate levels, the second order correction always pushes the levels apart, one goes up and one goes down. They "repel", a famous word in the context of this kind of discussion. Not clear how you would generalize this idea to more than two levels, probably there is a sum rule of some sort.

Further comments: I tried to make the connection between Saxon's approach and the general power series approach in all the details above. I was not really successful, since Saxon only treats degeneracy 2

and allows slightly non-degenerate states, which the other authors did not do. You have to decide which approach you are going to follow and then you get the results of that author in the symbols of that author.

6. Time-dependent perturbation theory (and transition probability and golden rule) (208)

[3.9.09] This is a pretty good 12 pages of Saxon dialog. As in Schiff, we write an expanded SE solution for $\psi(x,t)$ in terms of **coefficients** which can now vary in time. For Schiff they were $a_k(t)$, for Saxon they are $\mathbf{c_n(t)}$. The SE is recast in terms of the coefficients as in (61). The initial state is called k (in Schiff it was m). We compute $c_m(t)$ for ending up in state m starting in k as (62). First example is a constant H' (constant in time). All this does is shift our energy by H'_{kk} which agrees with first order SSPT. We can see that it does cause state transitions, since 62a is not zero. This is all just phasing stuff, but it does give the sinc form shown in (63). It you have some degenerate starting states, they get quickly mixed by this simple perturbation. Saxon is a little spooky in this section.

Page 211 then gets us into the notion of a **density of final states** (regardless of H'). We arrive at the **Fermi Golden Rule** (67) in the usual manner, though no delta functions are shown. We are reminded that H' has to be small in size for this rule to apply. Saxon does not assume sine perturbation form to arrive at this Golden rule and the sinc picture. My book would present this stuff in a different manner I think.

Now p 213 he assumes H' has $e^{\pm i\omega t}$ time dependence and we obtain the usual energy formula for absorption or emission of a photon, and he uses the terms **resonance absorption** and **stimulated emission**.

Page 214 reminds us that we are treating the field classically, but it is possible to treat it in QM as well. In this case, the zero point energy (vacuum) explains how ***spontaneous*** **emission** can occur! It would appear that it is a down transition stimulated by no field, but there is in fact a field there, and it all fits into the theory. That is to say, spontaneous emission fits into TDPT. It would be good to do a calculation on this subject at some point.

Saxon now does a **1D photo-ionization example**. He puts our electron into a narrow deep **1D well** with only 1 bound state of energy $-\varepsilon$ and whose ground state wavefunction has the form in (90). Various approximations are made to make this computation simple. The calculation is then done (first order TDPT using the golden rule) on page 218 with result (81). It seems odd to me that the rate goes to 0 as $\varepsilon \to 0$ and Saxon does not comment on this. I could figure it out if I had to. In terms of photon energy, you find that the rate drops as ω increases which also seems odd. You might think that the harder you hammer an atom, the higher transition rate you would get, but apparently not so. Probably due to kinematics. These questions are always hard to answer, even after you have derived an answer.

His final remark is that you can compute the rate per photon and that is a **cross section**.

Chapter VIII. Systems of Particles in 1D (227)

The subject of identical particles and symmetrization is wedged into this chapter. Obviously you have to be talking about multiple particles before this subject can come up.

1. Formulation. What does QM look like for multiple particles. This lays out what one expects. There is no factorization of the wavefunction, you just have $\psi(x_1, x_2, ...)$. Each particle has its own p and x operator. And you get the expected Hamilton's Ehrenfest type equations.

2. Two particles and CMS (229) Still in 1D and we assume $V(x_1-x_2)$ form for V. We separate into the relative coordinate x and the CMS coordinate X and end up with our reduced mass Hamiltonian as shown in (18). Schiff did all this as well. He points out that going from x_1 p_1 x_2 p_2 to x p X P is a Goldstein canonical transformation where I'll bet X is a cyclic coordinate and P a conserved momentum, but that detail is of little concern right at this point.

3. Interacting particles under uniform external forces. This just means redo the last section where not only do you have V(x), but some forces acting on the particles F_1 and F_2. This adds a term in (20) to the reduced μ equation. For gravity, these forces cancel and thus gravity does not affect QM. Electric field with opposite charges is another case that needs consideration (Stark) and these things are usually done by perturbation theory.

4. Coupled Harmonic Oscillators (236). So here is a prototype 2-particle problem with a coupling term as shown in 22. I will stop reading in this chapter at this point.

5. Weakly interacting particles with external forces. This is an application of perturbation theory.

IDENTICAL PARTICLES STUFF

6. <u>Identical</u> particles and exchange degeneracy. Obviously there will be degenerate states.

7. Systems of two identical particles (243).

8. Many-particle systems and Pauli Principle.(245). Yes, you can make fully symmetrized and fully antisymmetrized solution (write as Slater determinant page 50), one each. There are A! solutions if you don't do this, which is a LOT of solutions for large A. He then quotes the Pauli Rule as a simplification of nature. Bosons will have the fully sym, and Fermions the fully antisym. No proof of this is given, certainly. So OK, Saxon has now broached this important subject.

9. Systems of three identical particles. Writes out the sym and antisym solutions. Considers the triple coupled HO where all couplings have the same k. A good exercise.

10. Weakly interacting identical particles with external forces (255). If you do a two particle system and use the symmetrized states, energy expectation values then have those funny J and K direct and exchange integrals as I found doing X_2 molecule calculations a while ago.

Chapter IX. Motion in three dimensions (262)

This is more where I want to be *right now*, having read the first 5 chapters of Schiff. I just wanted to look at Saxon's *take* on all that stuff, but I thought it well to review Saxon up to this point, which I have just done, skipping the approximation methods stuff (which have not yet appeared in Schiff).

[first day of my walk ended here.]

1. Formulation: motion of one free particle. All 1D equations are generalized to 3D including flux and FT. The 2π factors continue to be equally distributed on the two sides of the transform. Form $e^{+\mathbf{p}\cdot\mathbf{r}/\hbar}$ is used for the plane wave.

2. V(r) separable in Cartesian coordinates. Separated functions works fine, each with its own E_i eigenvalues for i = 1,2,3. First example is particle in 3D box, three quantum numbers $n_1\ n_2\ n_3$. Shows energy diagram and notes that there is now a lot of state degeneracy: same energy for various n_i sets. You can compute the state density for such a box $\rho(E)$ as in (18). Second example is 3D HO which then has $3/2\hbar\omega$ in the ground state, and similar high degeneracy at higher levels. More degrees of freedom promote more degeneracy.

3. Central Potential: angular momentum eigenstates (268). Recall from curvilinear that

$$\nabla^2\psi = (1/\sqrt{g})\,\partial_i[g^{ii}\sqrt{g}\,\partial_i\psi] = (1/Q_1Q_2Q_3)\,\partial_i[\,Q_i^{-2}\,Q_1Q_2Q_3\,\partial_i\psi]$$

$$= (1/Q_1Q_2Q_3)\{\,\partial_1[Q_2Q_3/Q_1 * \partial_1\psi] + \partial_2[Q_3Q_1/Q_2 * \partial_2\psi] + \partial_3[Q_1Q_2/Q_3 * \partial_3\psi]\,\}$$

where in sphericals we know that $Q_r = 1$, $Q_\theta = r$, $Q_\varphi = r\sin\theta$. Recall that g_{ij} is the metric tensor (whose elements are Q_i^2 in this case), and g is its $\det(g_{ij})$. But Saxon's reader probably doesn't know all this curvilinear stuff, so a different method is used which I can state in terms of my transformation T matrix. Here think of unprimed as Cartesian and primed as Sphericals.

$$\partial/\partial x^i = (\partial\, x'^j/\partial x^i)\,\partial/\partial x'^j \qquad \text{or} \qquad \partial_i = T^j{}_i\,\partial'_j$$

Then one can manually compute the divergence like so:

$$\nabla^2 = \partial_i^2 = \partial_i\partial_i = [T^k{}_i\,\partial'_k]\,[T^j{}_i\,\partial'_j]$$

Saxon starts us off by computing one of the ∂_i , namely $\partial_x = T^j{}_x\,\partial'_j$, where we have to express the $T^j{}_x$ all in x' (ie spherical) coordinates to prepare for the next differentiation. This would take our student quite a long time!

So OK, we arrive at (24) and try the separated solution, get a separation constant β. We separate the Y and get another α.

Then we stop this and digress to write the angular momentum L_i first in Cartesians, and then in Sphericals. But how does the student do this? S/he has to start with $\mathbf{L} = \mathbf{r} \times \mathbf{p} = -i\,\mathbf{r} \times \nabla$ and is then faced with $L_i = -i\,\varepsilon_{ijk}\,x_j\partial_k$ and then has to use $\partial_i = T^j{}_i\,\partial'_j$ from above, and again convert things from prime to unprimed. So this is not really too bed

$$L_i = -i\,\varepsilon_{ijk}\,x_j\,T^j{}_k\,\partial'_j$$

My method of doing this is shown in " Angular momentum operators in spherical coordinates.doc" where I start by writing $\nabla = \hat{r}\,\partial_r + \hat{\theta}\,(1/r)\partial_\theta + \hat{\phi}\,(1/r\sin\theta)\partial_\phi$ to get

$$i\mathbf{L} = \mathbf{r} \times \nabla = \hat{r}\times\hat{\theta}\,\partial_\theta + \hat{r}\times\hat{\phi}\,(1/\sin\theta)\partial_\phi = \hat{\phi}\,\partial_\theta - \hat{\theta}\,(1/\sin\theta)\partial_\phi$$

Then I just dot this into the three Cartesian unit vectors like $\hat{\mathbf{x}}$ and the results fall out, and I quote

$$L_x = -i\,[\,\hat{x}\bullet\hat{\phi}\,\partial_\theta - \hat{x}\bullet\hat{\theta}\,(1/S\theta)\partial_\phi] = -i\,[\,(-S\phi)\,\partial_\theta - (C\theta C\phi)(1/S\theta)\partial_\phi] = i\,[\,S\phi\,\partial_\theta + \cot\theta\, C\phi\,\partial_\phi]$$

$$L_y = -i\,[\,\hat{y}\bullet\hat{\phi}\,\partial_\theta - \hat{y}\bullet\hat{\theta}\,(1/S\theta)\partial_\phi] = -i\,[\,(C\phi)\,\partial_\theta - (C\theta S\phi)(1/S\theta)\partial_\phi] = i\,[\,-C\phi\,\partial_\theta + \cot\theta\, S\phi\,\partial_\phi]$$

$$L_z = -i\,[\,\hat{z}\bullet\hat{\phi}\,\partial_\theta - \hat{z}\bullet\hat{\theta}\,(1/S\theta)\partial_\phi] = -i\,[\,(0)\,\partial_\theta - (-S\theta)(1/S\theta)\partial_\phi] = -i\,[\partial_\phi]$$

where Saxon has a factor of $\hbar$ since his L dimensions are physical, not dimensionless. Notice his ctn for cotangent which seems strange. He then computes L^2 and discovers that this combination is what appears in the angular separated equation. similarly, L_z appears in the azimuthal. We then conclude that separation constant β is going to be $\ell(\ell+1)$ and α is going to be m, but student does not know that yet.

Meanwhile, we can express $p^2/2m$ as shown in (40) which is just stating ∇^2 in sphericals. Saxon then does an interesting thing. Using a standard vector identity he arrives at (45) for L^2 by carefully maintaining the ordering of non-commuting x and p operators (but he then solves this equation for p^2) . He first notes that the classical version of this equation is $p^2 = (\hat{\mathbf{r}} \bullet \mathbf{p})^2 + L^2/r$ which certainly is similar looking. In any event, this (45) is then a way to write ∇^2 in terms of L^2 and one comments that the total linear momentum amplitude has a radial part and an angular part.

He next is forced to just quote the usual spherical harmonics results including the fact that β and α come out quantized. He does not say that these are normal eigenvalue equations that one just has to solve. That is, they are differential equations with some BC's in θ and φ which are pretty obvious.

When all the dust settles (as I like to say), we end up on page 275 with the eigenfunction of any central potential written with a radial function which solves 49 and we see the $(2\ell+1)$ degeneracy from m. He also quotes the $(-1)^\ell$ parity, and he notes the effective potential with a centrifugal term. He then writes $R = \chi/r = u/r$ in his case and the χ equation is 54 and it looks exactly like the 1D SE with this extra centrifugal term, and he says we need $\chi(r=0) = 0$ so that R = finite there. This means only the odd solutions of the 1D equation are allowed here, those that were sine like.

Saxon properly discusses the effect of the centrifugal term with some figures. On page 277 the V(r) is assumed to peak at r=0 and is so "repulsive". The "force" associated with this potential pushes away from r=0. You find the original V(r) curve looking at the ℓ=0 curve. Here, as ℓ increases, things just get more repulsive, there are no bound states. Figure 4 shows attractive, and there are now bound states for ℓ = 0,1,2 only in this example. The wavefunctions for ℓ = 0,1 might look as shown in Figure 5

4. Some examples. Example 1 is the **spherical square well** but only the ℓ = 0 solution. This is the same as our odd particle in box solution and you have some finite number of bound states. Saxon claims that you can think of the nuclear force as crudely corresponding to such a central square well. One can think of the deuteron as a bound state of the reduced mass n-p system. Studies show this is the only bound state of n-p, so this gives a rough idea of the depth of the square well, if you know its diameter a. If $a = 10^{-13}$ cm or so, the depth is a huge 40 MeV, huge on an electron scale of 1 eV.

Example 2 is **the HO** in 3D. He does not solve this here, but draws the energy level diagram sorted by values of ℓ . He keeps pointing out "accidental degeneracies", and here he associates this fact with another fact, that the problem can be solved in two different coordinate systems.

Example 3 is a **free particle**. The solutions are spherical Bessel functions $j_\ell(kr)$, he does not mention the n functions at all here, and we get some j_ℓ properties. In (66) Saxon quotes a fancy result which shows

how to expand a plane wave $e^{ik.r}$ in terms of the solutions in (65). Then for the particular $\mathbf{r} = r\hat{\mathbf{z}}$ this reduces to our usual e^{ikz} formula. You cannot have angular momentum about $\hat{\mathbf{z}}$ for such a wave, so m=0 in all the terms. That is to say, $L_z\, e^{ikr\cos\theta} = 0$ since $L_z = -i\partial_\varphi$.

5. The H atom. So we have now arrived here on page 286 with all tools in place. He does the usual Frobenius method in spherical coordinates, gets a recursion relation (75). He then just quotes the fact that the resulting polys are the associated Laguerres and then gives properties of these babies on page 289 including the generating function. We have radial and angmom quantum numbers n' and ℓ, but since n'+ℓ shows up a lot and in the energy, the "principle" quantum number n is defined, and we end up with the usual basic situation of atomic physics. The degeneracy of an energy level is n^2 and we have states of different ℓ having the same energy. Once again (about the 4th time) he mentions this is an accidental degeneracy and "it arises from the fact that you can separate things in parabolics". He does not give any hint of why that reason should convince a student, and he says nothing about O(4) symmetry, so I am still looking for a discussion of this somewhere. All in all, a good section for the intended audience: all the key results are quoted.

Chapter X. Angular Momentum and Spin (298)

1. Orbital L (298). Using the [x,p] commutator, Saxon derives the usual L_i commutator in $\mathbf{L}\times\mathbf{L} = i\hbar\mathbf{L}$ notation, I have not seen ε_{ijk} in this book. He then shows that $[\, L^2, \mathbf{L}\,] = 0$. Results generalized to multiple particles. Finally, looks at the CMS + Relative motion decomposition, each has an L that satisfies its own rule, no cross commutator, so completely independent. An interesting point.

2. Eigenfunctions and eigenvalues. States the two eigenvalue equations with unknown eigenvalues α and β, then constructs L_+ and L_- and using these, shows there is an L_z ladder of states which must terminate at each end. And with more fiddling (there is a lot of it), gets the usual $\ell(\ell+1)$ and m results as stated in (30) page 305. So I think this would make the student quite pleased to see this all done a priori.

Generalizes the results to any J or S or whatever that satisfies the comrels.

Makes the point that 2π rotation can give -1 at the same point, so can have two phases as with the half integral ℓ values, does not violate any QM rule. But all states of a given system just either be integral or half-integral. A reason is given that otherwise, you would get interference effects if the same system could have two states of different half-integrality. That is to say, if you made a lincomb you could show that the same point in space had two different values of $|\ |^2$ which is not legal. If you do a 2π rotation, all half-integral states to go minus, but he does not reference this fact.

Next, he asks what the UP has to say about J ? The conclusion seems to be that $\langle J^2\rangle \geq \langle J_z^2\rangle$. We then get to the cone pictures that Levitt does not like. The angle of a cone must be this

$\cos\theta = m/\sqrt{j(j+1)}$ and the top cone has $\cos\theta = j/\sqrt{j(j+1)}$ so $\theta > 0$.

The cone picture I guess shows that when J_z has a specific value, then $\langle J_x\rangle = \langle J_y\rangle = 0$. Not clear how he proves this fact.

Finally, again using $L_\pm$, he creates a Rodriguez formula for the spherical harmonics as on p 313.

3. Rotation and translation operators. He first shows that L_z is the $R_z(\varphi)$ generator and goes from the infinitesimal to the finite rotation using the famous limit rule which he shows is just the power series e^x obtained from a binomial expansion. He then claims a generalized result for $\hat{\mathbf{n}} \bullet \mathbf{L}$ instead of just L_z. The, if L commutes with H, any rotation of a solution gives another solution to the problem, etc. He then mentions the translation operator being p and the finite translation operator being $T_z(\mathbf{a}) = \exp(i\mathbf{a} \bullet \mathbf{p})$, so if H commutes with p, then any translated solution is also a solution. And in the first case, L is a constant of the motion (at least L^2 and L_z are), and in the second case **p** is a constant of the motion. Thus we connect symmetry with commutator with H with something being conserved.

4. The Pauli Operators. A nice opening free discussion on "spin" and no classical limit. No mention of Casimirs of SO(3.1). Crude $\ell \oplus 1/2$ rule. He then goes on to have a sort of direct product state, uses χ for spinor states, he is talking only spin 1/2 here. Basically $\mathbf{S} = \hbar/2\ \boldsymbol{\sigma}$, the matrix representation. Comment that Pauli introduced this to explain experiment, but in 1930 Dirac's relativistic electron theory made spin appear directly.

5. Adding Angular Momenta. The claim is that there is a general solution (77) with CG coefficients, and that the range of resulting j is as we know it. Add up states wither way and get the same number as page 330. Comment on L-S versus j-j coupling in atoms. Then he finds the states for combining two spin 1/2 spins. He then writes the J eigenstates for the $\ell \oplus 1/2$ situation. For $\ell \oplus 1/2$ states are as in (90) where you just let m take its natural values, the other in (91). These combination space-spin states are the ones you would use for handling an **L•S** coupling perturbation since **L•S** commutes with L^2, S^2 and J^2 and J_z. The form of the LS coupling is shown bottom page 335 and is presented in BD I page 51 in the FW chapter. The dV/dr arises because electric field E is sitting there. So here |JM; LS> would be the kind of states you want and then the L•S coupling splits them apart in an obvious manner. But Saxon stops short of "doing atomic physics" here.

Chapter XI. Applications and Further Generalizations (344)

1. The Helium Atom and the Periodic Table. I spoke too soon! Write H for two electron atom, assume separation for starting position, so assume each in 1S with simple wavefunction (3). Then the energy shift is $\langle\varphi|H'|\varphi\rangle$ as in (5). But how do you do that fancy double integral? A Jacksonian method and its result is quoted. This method gives the second column of energies in the table on page 347 and is not really too far off experimental results. The results are improved using a variational Z' idea which is Rayleigh-Ritz and we get the third column which is then very close.

So this was with both electrons in the ground state. If one has bumped up to some excited state, it then has some $\psi_{n\ell m}$ while the other is still ψ_{100}. We then have to plug these states into (5) to get the adjusted energy from first order perturbation theory. This then involves those famous J and K integrals called Coulomb and Exchange shown page 348. Results are not given.

Now along comes spin. The ground state just mentioned is $(1S)^2$: the space state is sym, so the spin state is antisym (fermions), so S = 0 singlet. This is the lower left state page 349 figure, called $^1S_0$. Since no L yet, J = S = 0. EM transitions tend not to change S, so you then have two distinct classes of states, the famous para and ortho helium. In this case, triplet spin states have antisym space states, the electrons stay further apart, energy is lower, hence Hund's Rule: triplets lie below singlets, as suggested in the figure.

Saxon goes on to do more "atomic physics" and builds a little periodic table page 351. I have not read this in detail today, but will when the time comes for "atomic physics".

2. Theory of Scattering. Finally this topic appears! We get lots of talk, then the starting position in (17). Then come the two fluxes and the cross section as in (18). A clear statement " cross sections provide our main knowledge about elementary particles". We then have the radial equation assuming V(r), we already know $j_\ell(kr)$ for this problem if V(r) = 0 with sine limit as shown, and we assume the V(r) induces some phase shift as in (21). The argument is that V cannot change the general asymptotic form, so all it can do is induce a phase shift. A more detailed arg is made by me that you get mix of j_ℓ and n_ℓ etc. He then just quotes the partial wave series for f(θ) as in (22). He does not do the "balancing act" which results in this form, just says "it follows that", and probably this is why I have been long unhappy with my scattering partial wave stuff. Schiff cleaned all this up for me so I am now happy with (22). He goes on then to do the total cross section form, and then the optical theorem for the forward direction. Claims the optical theorem is very general as did Schiff. He goes on to show that at low energy, only a few partial waves will be activated.

He now comments on the Coulomb case on page 358. He just quotes the Schiff result for $f_c(\theta)$, and shows that we get the Rutherford formula and comments that this is a pretty amazing fact that there is no quantum effect at all. But for identical particles, he then shows that you do get phase effects [he says you need to add the exchange amplitude for bosons, we presume to make a sym space wavefunction] and then you would see quantum effects, and we see why these would go away for large n. All very clear. He even quotes the identical particle cross section formulas which I have not yet seen in Schiff (I am there at the end of Chapter 5 only).

3. The Born Approximation. Skipped.

4. Motion in an EM Field. He quotes the classical Hamiltonian for a particle in an EM field in (59a), and then looks at Hamilton's equations to notice that p is no longer ma, but π is. We imitate the classical H to write the QM H as in (63). Doing a gauge transform to clean things up, we get to (67) for the Ham where script H is a B field and this leads to the idea that the electron has a mag moment as on page 376. We then have the gyro ratio discussion and how it is 2 for an electron relative to the orbital 1. So this section mainly arrives at the $-\boldsymbol{\mu}\bullet\mathbf{B}$ Hamiltonian terms as in NMR.

5. The Dirac Theory of the Electron. I buzzed through this just now, being an expert at the moment, it is a good discussion and hits all the key points. The argument for linear ∂_t and the relativity says linear ∂_x and then you are forced to 4x4 matrices and then you are forced to include negative energy states, and then out comes the positron and spin etc. The Lamb shift does not come out because the EM field here is not quantized. My head must have spun when I read this section.

6. Mixed States and the Density Matrix. A good topic to include, and I won't read it since I just did Levitt and learned all about this stuff and have it written up elsewhere.

Appendix I: Gaussian Integrals (397)

These integrals arose in the discussion of Gaussian wave packets, and perhaps in the HO discussion, so he just gathered it all right here.

Normally a book like this might have LOTS of appendices where details are shoved. Saxon did not do it that way, his details were all handled "in line".

Appendix II: Selected References (400)

He lists off 30 books, of which I have 8 in the 457 Library. Gives Dirac's book the maximal rating.