Schiff Quantum Mechanics 3rd Ed 1968 PhL 11.12.07

reviewed and comments added on 12.26.08

This document contains notes only on Schiff Chapter 6. He makes a distinction between "representations" such as |r> and |k>, and "pictures" such as the Heisenberg picture.

He starts with a matrix math review in **Section 22**.

Then in **Section 23** he talks about "transformations between representations" such as W and U and V, and he introduces the idea of a state vector in Hilbert Space and the bra-ket notation.

In **Section 24** he writes down the "equations of motion" in the three "pictures". He then relates the Heisenberg picture to classical mechanics with its Poisson Brackets. The system of a non-relativistic non-quantum particle interacting with a classical EM field is treated briefly to show how you might move from classical system to a quantum system. The "first quantization" requires the replacement of the Poisson Brackets with a commutator and some proper ordering of things. He thus ends up with the quantum Hamiltonian shown at the bottom of page 179. This section ends with comments on the virial theorem which I skipped.

Then finally in **Section 25** he solves the 1D harmonic oscillator system using matrix mechanics. He does this in the "energy representation" and the "Heisenberg picture" in which the states don't move.

Chapter 6: Matrix Formulation of Quantum Mechanics 2

Section 22 Matrix Algebra (149) 2

Matrix Add and Multiply (149) 2

Trace, Determinant, Inverse (151) 2

Hermitian and Unitary Matrices. (152) 2

Transformation and Diagonalization of Matrices (152) 2

Functions of matrices (153). 3

Matrices of infinite rank (153). 3

Section 23 Transformation Theory (155) 3

Unitary matrix W. (155) 4

Transformation of the Hamiltonian with W (156). 4

Transformation of the Hamiltonian with U (157). 5

Transformation of the Hamiltonian with V (159). 6

Representations of Operators (159). 7

A Useful Identity (160) 7

Row and Column matrices (161). 7

Hilbert Space (163). 8

Dirac's Bra and Ket Notation (164) 8

Projection Operators (166). 8

Physical meaning of matrix elements (167). 8

Section 24 Equations of Motion (167) 9

Schrodinger picture (168) 9

Heisenberg picture (170). 9

Interaction picture (171) 10

Energy Representation (173). 10

Classical vs Quantum Theory (173) 10

Poisson vs Commutator Brackets (175). 10
Quantization of a Classical System (176). 11
Motion of a particle in an EM field (177). 11
Evaluation of commutator brackets (177). 13
Velocity and acceleration of a charged particle (178). 13
Virial Theorem (180). 13
25. Matrix theory of a harmonic oscillator (180). 13
Energy Representation (181). 13
Raising and lowering operators (182). 14
Matrices for a, x and p (183). 14
Coordinate representation (184). 14
Summary of Chapter 6: 14
Test Question #1 14

Chapter 6: Matrix Formulation of Quantum Mechanics

Section 22 Matrix Algebra (149)

Matrix Add and Multiply (149) Nothing new here

Trace, Determinant, Inverse (151)

tr(ABC) = tr(BCA) etc.
det(AB) = detA detB
$(AB)^{-1} = B^{-1}A^{-1}$

Hermitian and Unitary Matrices. (152)

$B = A^{\dagger} = (A^T)^*$ is the hermitian adjoint of matrix A
$(AB)^{\dagger} = B^{\dagger}A^{\dagger}$
A hermitian matrix is one that equals its adjoint $A^{\dagger} = A$, can only be square
$U^{\dagger} = U^{-1}$ defines a unitary matrix,

Transformation and Diagonalization of Matrices (152). A "transformation of A by S" is written as $SAS^{-1} = A'$. The matrix S is of course invertible by definition, and M&M call S a "similarity transformation". If you write any "matrix equation" then transform all the matrices, the equation keeps its form, so like a change in basis somehow. Note that det(A) = det(A') and tr(A) = tr(A'). [det = norm!]

A diagonal matrix's diagonal elements are the eigenvalues of the matrix. Powers of diagonal matrices are diagonal with powered eigenvalues. When we write $SAS^{-1} = A'$ and get A' to be diagonal, then A was "diagonalizable by S" and we could write SA = A'S. If we call the diagonal elements of A' by the name λ_k, then easy to show that $SA = A'S \Rightarrow S(A-\lambda_k I) = 0$ for each k. If the matrix $(A-\lambda_k I)$ is invertible, then S = 0 which contradicts our assumption that we have an S such that $SAS^{-1} = A'$. Thus, it must be true that $\det(A-\lambda_k I) = 0$ for each λ_k. The equation $\det(A-\lambda I) = 0$ with λ a free parameter is called the **secular equation**. It is a polynomial of degree N in λ and it has N roots λ_k [see 12.21]. Thus, one way to find the N eigenvalues of a diagonalizable matrix A is to find the N roots of $\det(A-\lambda I) = 0$. Suppose you do another transformation $B = Q^{-1}AQ$. Notice that $\det(B-\lambda I) = \det(Q^{-1}[A - \lambda I]Q) = \det(A-\lambda I)$. This says

that the polynomial in λ det(B-λI) is exactly the same as the polynomial in λ det(A-λI), so the equation det(A-λI) = 0 will have the same roots as the equation det(B-λI) = 0. This shows that the eigenvalues of a diagonalizable matrix are invariant under similarity transformation. If there are several matrices that diagonalize A according to $SAS^{-1} = A'$, it is clear that the eigenvalues are the same for any S since the secular equation does not involve S.

Interesting closing comment which I have verified. If a matrix equation involves A and $A^\dagger$, then the equation form is only preserved by a transformation S which is unitary. In this case, $(A')^\dagger = (A^\dagger)'$ which makes things work out right.

Functions of matrices (153). If f(A) is a convergent series, everything works out in the obvious way. Then he quotes the famous result $\det(e^A) = e^{tr(A)}$. The proof of this is not quite trivial, and I have a good proof as "item 4" in my Matrix Notes which is now the last section of my Matrix Binder.

Matrices of infinite rank (153). You can think of either index as becoming a continuous variable and summation becomes integration and all that stuff. At this point, he quotes two very famous theorems:

T1: Any hermitian matrix can be diagonalized by a unitary transformation [there may be more than 1] .

This says we can do our $SAS^{-1} = A'$ trick for any hermitian A, and this implies from above that the eigenvalues are unique since the secular equation has only one set of solutions. In other words, a hermitian matrix has a unique set of eigenvalues if eigenvalues are defined (as they were here) as the diagonal elements of the diagonalized matrix. [not sure I have a complete proof of this]

T2: $[A,B] = 0 \Leftrightarrow$ A,B can be diagonalized by the same unitary transformation

I have shown this in my "physics questions" and there is help from a web page referred to there.

Schiff then gives a quick proof that all eigenvalues of hermitian matrix A are real. And the *converse*: a diagonalizable matrix with real eigenvalues is hermitian.

He closes with a warning that you have to check both left and right inverses (or adjoints) before you can say you have an inverse or adjoint (when dimension is infinite I think).

Section 23 Transformation Theory (155)

In the opening paragraphs, we just write the usual coordinate-space SE as $H_{op}\ u_k(r) = E_k\ u_k(r)$ where H_{op} includes differential operators. This is the time independent SE and it was developed in earlier chapters of the book, so reader is happy to accept this thing. I think he should be saying something here like the set of functions $u_k(r)$ span the space $f:R^3 \rightarrow R^3$ (normalizable), that is, they form a complete orthonormal set.

Comment: In the following three subsections we examine unitary transformation matrices W,U and V. Each of these "links" two of the three representations which I will call energy, coordinate, and arbitrary. The diagonal operators in the three cases are H, R and Ω. The linkage matrix is always unitary if in each space you have a clean identity representation for "1", that is, normalizations are preserved. In each representation, we can choose to look at matrix elements of the Hamiltonian H operator if we want to. In the case of U which links energy and coordinate space representations, the columns of $U^\dagger$ are eigenfunctions. This seems now like a lot of aimless shuffling around, maybe Schiff is just trying to get

the reader familiar with the infinite matrix idea. Well, I think he wants to develop a reservoir of complex looking equations which then all simplify when he does the bra ket notation on page 165

Unitary matrix W. (155). Here we consider some other operator Ω which has its own separate set of eigenvalues ω_μ and eigenfunctions $v_\mu(r)$. To help us out, he now has Greek indices. This set of functions is also complete, so the claim is that you can express a function in one set as a lincomb over the other set as shown in (23.4). He shows that W must be a unitary matrix and here is my bra-ket proof:

$W_{m\mu} = \langle m|r\rangle\langle r|\mu\rangle$ and thus $(W^\dagger)_{\mu n} = (W_{n\mu})^* = \langle n|r'\rangle^*\langle r'|\mu\rangle^* = \langle\mu|r'\rangle\langle r'|n\rangle$. Therefore

$[\, WW^\dagger \,]_{mn} = W_{m\mu}\,(W^\dagger)_{\mu n} = \langle m|r\rangle\langle r|\mu\rangle\,\langle\mu|r'\rangle\langle r'|n\rangle = \langle m|n\rangle = \delta_{m,n}$

where we use completeness three times in the second last equality. I think he has basically shown that if you have two sets of complete orthonormal basis functions over a Hilbert space, they are related by a unitary transformation. I could go look this up in Stakgold Hilbert Space stuff, but I am happy as is.

Well, here is a faster path for the above:

$W_{m\mu} = \langle m|\mu\rangle$ and thus $(W^\dagger)_{\mu n} = (W_{n\mu})^* = \langle n|\mu\rangle^* = \langle\mu|n\rangle$, so we get

$[\, WW^\dagger \,]_{mn} = W_{m\mu}\,(W^\dagger)_{\mu n} = \langle m|\mu\rangle\,\langle\mu|n\rangle = \langle m|n\rangle = \delta_{m,n}$ hence $WW^\dagger = 1$

Notice that W is not some arbitrary matrix, it is *the* matrix (or at least *a* matrix) that connects the energy representation of H to the representation of operator Ω. Again, $W_{m\mu} = \langle m|\mu\rangle$. That is, W moves you from the representation in which H is diagonal, to the one in which Ω is diagonal.

Note added 12.26.08: Here is an example. Consider the transformation between the 3D momentum and the 3D coordinate space representation:

$W_{\mathbf{pr}} = \langle \mathbf{p}|\mathbf{r}\rangle = e^{i\mathbf{p}\bullet\mathbf{r}}$ $\quad W^{-1} = e^{-i\mathbf{p}\bullet\mathbf{r}} = W^* = W^{*T} = W^\dagger$ $\quad \Rightarrow \quad$ W = unitary.

Transformation of the Hamiltonian with W (156). Reminder: W is the unitary matrix $W_{m\mu} = \langle m|\mu\rangle$ which links the energy or H representation |m> to the Ω representation |μ> with $v_\mu = \langle r|\mu\rangle$ eigenfunctions, where Ω is some arbitrary Hermitian operator.

For the first time, Schiff writes the Hamiltonian *matrix* elements like this: [where k and ℓ are energy eigenstates]

$H'_{k\ell} = \langle k|r\rangle\,[\, H_{op}\langle r|\ell\rangle\,]$ where H_{op} is our familiar coordinate-space differential operator on r.

so H' is the matrix in the energy basis. In the other basis (Greek υ basis) you could similarly write:

$H''_{\mu\upsilon} = \langle\mu|r\rangle\,[\, H_{op}\langle r|\upsilon\rangle\,]$ with same H_{op}. Now we get a different matrix H".

Now calculate:

$$(WH''W^\dagger)_{mn} = W_{m\mu}\, H''_{\mu\upsilon}\, (W^\dagger)_{\upsilon n} \qquad = \langle m|r''\rangle\langle r''|\mu\rangle \langle \mu\,|r\rangle\, [\, H_{op}\langle r|\upsilon\rangle\,]\ \langle \upsilon|r'\rangle\langle r'|n\rangle$$
$$= \langle m|r\rangle \quad [\, H_{op}\langle r|\upsilon\rangle\,]\ \langle \upsilon|r'\rangle \quad \langle r'|n\rangle$$
$$= \langle m|r\rangle \quad H_{op}[\, \langle r|\upsilon\rangle \langle \upsilon|r'\rangle \langle r'|n\rangle\,]$$
$$= \langle m|r\rangle \quad H_{op}[\, \langle r|n\rangle\,]$$
$$= H'_{mn}$$

which shows that $WH''W^\dagger = H'$. But in our basis functions $\langle r|m\rangle$, H' is diagonal

$$H'_{k\ell} = \langle k\,|r\rangle\, [\, H_{op}\langle r|\ell\rangle\,] = \langle k\,|r\rangle\, [\, E_\ell \langle r|\ell\rangle\,] = E_\ell \langle k\,|r\rangle\langle r|\ell\rangle = E_\ell \langle k\,|\ell\rangle = E_\ell\, \delta_{k,\ell}$$

So, if we have a Hamiltonian matrix H" in some weird basis [operator Ω], there will be some unitary transformation W that will take it to the diagonal basis. We then have a new way to solve the SE:

(1) compute $H''_{\mu\upsilon} = \langle \mu\,|r\rangle\, [\, H_{op}\langle r|\upsilon\rangle\,]$ in some arbitrary basis associated with some operator Ω

(2) find W that brings H" to diagonal form $WH''W^\dagger = H'$. You then know the eigenvalues as the diagonal elements of H', and the eigenfunctions are given by the elements of vector U [recall V=UW so that $U = VW^\dagger$] . We can write this last thing out as

$\langle r \mid k\rangle = \langle r|\mu\rangle \langle \mu \mid k\rangle$ red comments here seem out of place.

We can recap what we just did in the language of the previous matrix sections. We know that the Hamiltonian matrix H is hermitian matrix because its eigenvalues we know are real. Therefore we know we can diagonalize H" by a unitary transformation. So doing $WH''W^\dagger = H'$ is no surprise. [That is to say, H" was not diagonal with the H' eigenfunctions.] The key thing Schiff has done is tie this matrix stuff to the coordinate-space operator H_{op} that the student already knows about.

Since observables have real eigenvalues, we know that the operator for any observable is hermitian.

Transformation of the Hamiltonian with U (157). Reminder: U is the unitary matrix $U_{rm} = \langle \mathbf{r}|m\rangle$ which links the energy or H representation $|m\rangle$ to the coordinate **R** representation $|\mathbf{r}\rangle$. So U is a particular example of W where we set $\Omega = \mathbf{R}$.

Now we sort of start over. The unitary matrix U is not just *any* unitary matrix, it is one that takes your coordinate-space SE Hamiltonian to diagonal form, $UHU^\dagger = H'$ (= diagonal). The matrix elements of U have the form $U_{kr} = \langle k|r\rangle$ as shown in (2) below, so think of U as connecting the SE (energy) representation (Latin letters like k) with the coordinate space representation).

There are two interesting points made in this section:

(1) Equation (23.13) at first seems odd, but here it a derivation. Recall from above that

$$H'_{k\ell} = \langle k\,|r\rangle\, [\, H_{op}\langle r|\ell\rangle\,] = \langle k \mid H \mid \ell\,\rangle$$

Then

$$\langle r \mid H \mid r'\,\rangle = \langle r \mid k\,\rangle \langle k \mid H \mid \ell\,\rangle\langle \ell \mid r'\,\rangle = \langle r \mid k\,\rangle H'_{k\ell} \langle \ell \mid r'\,\rangle$$

$= \langle r \mid k \rangle \langle k \mid r'' \rangle [\, H''_{op} \langle r'' \mid \ell \rangle \,] \langle \ell \mid r' \rangle$

$= \langle r \mid r'' \rangle \; H''_{op} \; [\, \langle r'' \mid r' \rangle \,]$

$= \delta(r-r'') \; H''_{op} \, \delta(r''-r')$ which is still integrated over r'', so

$= H_{op} \, \delta(r-r')$ // and this is (23.13)

If H_{op} had no differential operators, then $\langle r \mid H \mid r' \rangle$ would be a "diagonal" matrix, but it does have these operators so H is not diagonal in the coordinate-space basis (but it is zero any finite distance away from the diagonal!)

(2) If you can diagonalize H with some unitary U: $UHU^{\dagger} = H'$ (= diagonal)

then you conclude (see text) that the traditional (coordinate space) eigenfunctions of H are given by

$u_k(r) = (U^{\dagger})_{rk} = U_{kr}^*$ or $u_k(r)^* = \langle k|r \rangle = U_{kr}$

Notice that each row in the matrix U is labeled by k. Thus, the eigenfunctions (starred) are the rows of the matrix U. The eigenfunctions are also the columns of $U^{\dagger}$. Again: the eigenfunctions of a problem [system with hermitian Hamiltonian H, eg] are the columns of the unitary matrix $U^{\dagger}$ which brings H to diagonal form, and the diagonal elements are then the eigenvalues. [This is just an old matrix fact, really.]

The fact that U is unitary is pretty obvious:

$(UU^{\dagger})_{k\ell} = U_{kr} \, U_{\ell r}^* = u_k(r)^* \; u_{\ell}(r) = \langle k|r \rangle \langle r|\ell \rangle = \langle k|\ell \rangle = \delta_{k\ell}$

$(U^{\dagger}U)_{rr'} = U_{kr}^* \, U_{kr'} = u_k(r)^* \; u_k(r') = \langle k|r \rangle \langle r'|k \rangle = \langle r'|k \rangle \langle k|r \rangle = \langle r'|r \rangle = \delta(r-r')$

Notice that you would not call matrix U "square" since it has a discrete spectrum index on one side and a continuous one on the other side (the H spectrum versus the R spectrum). But both H's are square. And recall Schiff's earlier comment that you want to show both $UU^{\dagger} = 1$ and $U^{\dagger}U = 0$ which is shown above.

Transformation of the Hamiltonian with V (159). In the last section, we had a matrix U which connected the energy to the coordinate space representation. In the same manner, we could have made a matrix V which connects the Ω operator representation to the coordinate-space representation. Compare:

$UHU^{\dagger} = H'$ U connects r-space (H) to E-space representation (H')

$VHV^{\dagger} = H''$ V connects r-space(H) to Ω-space representation (H'')

But in our first section, we had

$WH''W^{\dagger} = H'$ W connects Ω-space(H'') to E-space(H') representation

Putting this together we are not surprised to learn that

$W = U V^{\dagger}$ as shown in (23.18). so $U = WV$ and $V = W^{\dagger}U$

Remember that U,V,W are each matrices, not vectors. It is good to write things like this:

$V^{\dagger} = U^{\dagger}W$ and $U^{\dagger} = V^{\dagger}W^{\dagger}$

Remember that the eigenfunctions are the columns of $U^{\dagger}$ or $V^{\dagger}$. So these equations tell you how to get from one set of eigenfunctions to the other. You right-multiply by W or $W^{\dagger}$.

Representations of Operators (159). This text summarizes what we have done above, how we have now looked at the Hamiltonian H in three different representations which I call |r>, |k> and |μ>.

A Useful Identity (160) . First, here is equation (23.20) :

LHS = $\langle\alpha|\, r\rangle\, \Omega_{op}\, [\langle r|\beta\rangle]$ but write $\Omega_{op}\, [\langle r|\beta\rangle] = \langle r \mid \Omega \mid \beta\rangle = \langle r \mid \Omega \mid r'\rangle\langle r'|\beta\rangle$

so LHS = $\langle\alpha|\, r\rangle\, \Omega_{op}\, [\langle r|\beta\rangle] = \langle\alpha|\, r\rangle\langle r \mid \Omega \mid r'\rangle\langle r'|\beta\rangle = \langle\alpha|\, r\rangle\, \Omega_{rr'}\, \langle r'|\beta\rangle$ = RHS

Can rewrite the RHS as this:

RHS = $\langle r'|\beta\rangle\, \Omega_{rr'}\, \langle\alpha|\, r\rangle = \langle r'|\beta\rangle\, \Omega^{\dagger *}_{r'r}\, \langle\alpha|\, r\rangle = \Omega^{\dagger *}_{r'r}\, \langle r|\alpha\rangle^{*}\, \langle r'|\beta\rangle = [\Omega^{\dagger}_{r'r}\, \langle r|\alpha\rangle]^{*}\, \langle r'|\beta\rangle$

Now suppose we make this operator definition [really same was we handled Ω_{op}]

$\Omega^{\dagger}_{op}\, \langle r|\alpha\rangle = \langle r|\Omega^{\dagger}|\, r'\rangle\langle r'|\alpha\rangle = \langle r \mid \Omega^{\dagger} \mid \alpha\rangle = \Omega^{\dagger}_{rr'}\, \langle r'|\alpha\rangle$

Then

$\Omega^{\dagger}_{r'r}\, \langle r|\alpha\rangle = \Omega^{\dagger}_{op}{}'\, \langle r'|\alpha\rangle$

so that

RHS = $[\Omega^{\dagger}_{r'r}\, \langle r|\alpha\rangle]^{*}\, \langle r'|\beta\rangle = [\Omega^{\dagger}_{op}{}'\, \langle r'|\alpha\rangle]^{*}\, \langle r'|\beta\rangle = [\Omega^{\dagger}_{op}\, \langle r|\alpha\rangle]^{*}\, \langle r|\beta\rangle$

so we have now shown that

$\langle\alpha|\, r\rangle\, \Omega_{op}\, [\langle r|\beta\rangle] = [\Omega^{\dagger}_{op}\, \langle r|\alpha\rangle]^{*}\, \langle r|\beta\rangle$ (23.21)

Where both Ω_{op} and $\Omega^{\dagger}_{op}$ are differential operators. If Ω is hermitian, they are the same. This gives you a way to operate on $\langle r|\alpha\rangle$ if you don't like operating on $\langle r|\beta\rangle$. This is "the useful identity". Comment: he is just getting the Hilbert Space "adjoint operator" defined in this particular representation.

Row and Column matrices (161). In (23.24) you can think of ψ_{α} as a column vector whose components are labeled by r values, which I would call $\langle r|\alpha\rangle$. But define $a_{\alpha} = \langle k|\alpha\rangle$ as the same HS vector but we

are now looking at its components in the energy space. Think of $|\alpha>$ as a vector and we are projecting it onto different choices of axes, the $<k|$ choice or the $<r|$ choice. We know we can write

$<k|\alpha> = <k|r><r|\alpha>$ and we know that $<k|r> = U_{kr}$ from above, so

$<k|\alpha> = <k|r><r|\alpha>$

$a_\alpha = U \psi_\alpha$ vector = matrix * vector

The U matrix takes an arbitrary vector from the coordinate representation to the energy representation. Recall from $UHU^\dagger = H'$ that this same matrix U took the Hamiltonian from the coordinate to the energy representation. In one case we are working on an operator like H, in the other case on a vector .

Final comment is that unitary transformations like U don't change the normalization.

Hilbert Space (163). The geometric picture is this: a state like $|\alpha>$ is a vector in a Hilbert Space and you can select any set of axes in the space that you want, such as the $<k|$ choice or the $<r|$ choice. Schiff does not define a Hilbert Space, but I know it is in inner product space with the "natural metric" and it has to be complete -- no pieces are somehow missing. So now all our operations I have been writing as $<a|b>$ can be understood as the inner products in this space. A transformation like U "rotates the axes" of the space, leaving the vector like $|\alpha>$ put. The Hilbert Space is closed under actions by our hermitian operators like Ω , so think of those as "generalized rotations" where length can change too.

[More on these "axes": imagine a 1D QM problem with $\psi(x)$ as the solution, or $<x|\psi>$. Each *point* on the real axis x in R^1 is itself an "axis" in our HS. Since there are an infinite number of points on the x axis, there are an infinite number of axes in the HS. The component of ψ on "axis x" is $<x|\psi>$. Notice the potential confusion between "the x axis in R^3" and "the axis x in the HS". { Note added: a mapping that takes one function f(x) into some other g(x) just changes the weights on the set of x "axes". In general, this change of weights won't be unitary. }

Now, when you "rotate the axes" to the energy representation, you still have an infinite number of axis, but now each one is represented by $<k|$ where k is no longer (for bound state problems) a continuous variable. But there are (may be) an infinite number of eigenvalues E_k so there are still an infinite number of axes. It is a little hard to picture the rotation of the axes in HS, but the idea I think is sound.]

Dirac's Bra and Ket Notation (164). Completely understood, nothing to say. The $|\alpha>$ is a vector in the Hilbert space, whereas $<\beta|$ is a vector in the adjoint space I think, but that term is not used here. All the equations earlier are now written in their compact form. So we have moved from QM in the coordinate representation, to QM in the abstract Hilbert space with its abstract operators, where we want to be!

Projection Operators (166). Define $P_\mu = |\mu><\mu|$. This is a component of unity since if you sum you get 1. You have projected out of unity the contribution of state or axis μ. P_μ is an operator and a matrix. It has lots of useful properties that are given here, but I don't care about this right now, so move on. I will come back right are when the time is right, which will probably be soon since these are used in spin work a lot. (this will play a role in the density matrix formalism)

Physical meaning of matrix elements (167). We can interpret diagonal elements of a matrix like $<\alpha|\Omega|\alpha>$ as the expectation value for the quantity represented by operator Ω when system is in state α

(assuming α is normalized). So diagonal elements are expectation values, but off-diagonal elements are harder to interpret. We shall see off-diagonals later in certain cases as transition amplitudes.

Section 24 Equations of Motion (167)

This is the section I have been aiming at, and I plan to do a solid review of it right here. This is about the various "pictures" and the SE written in Hilbert Space and the role of commutators, and the linkage to classical mechanics. [resuming here 11.14.07]

The words in the opening text are very good. Since they all "make sense", I know I understood the earlier sections. The new comment here is that everything was at some one instant of time. If we had some Hamiltonian H_{op} that was really $H_{op}(t)$, then we have to imagine that *everything* changes in time, all the basis functions move, the matrices move, and so on. So our whole discussion was at some $t = t_1$.

As things move in time, you can think of it in three ways, and these will be the three "pictures" : the state vector moves, the axes move, or they both move!

Schrodinger picture (168) . All very simple. (24.1) shows how a state vector moves under the force of the Hamiltonian which at this point is assumed NOT to depend on time. The state vector nevertheless DOES depend on time, and that is what the TDSE says, which is what (24.1) is. Notice the key minus sign that you get from the "i" factor when you make the bra move in time rather than the ket.

The solution for time independent H is the exponential form (24.3), and now we have a genuine application with an exponentiated operator. Earlier it seems like a cute mathematical oddity, but here it is in the real world, in action.

Now we come to (24.4) which tells how an operator Ω changes in time when sandwiched between some states. Notice that the states have the "S" label since they are in the Schrodinger picture. There are three terms from the derivative, and the minus sign just noted above causes the commutator to appear, so now for the first time we see a commutator in action. Here is the equation:

$$d/dt\ [\ <\alpha_S(t)\ |\ \Omega_S(t)\ |\ \beta_S(t)>\ ]\ \ =\ \ <\alpha_S(t)\ |\ \{d/dt\ \Omega_S(t)\}\ |\ \beta_S(t)> + <\alpha_S(t)\ |\ [\Omega_S\ ,\ H]\ |\ \beta_S(t)>/(i\hbar)$$

So, if Ω_S itself does not change in time, then the matrix element's time change is driven by the commutator as shown. And if the Ω_S commutes with H as well, then Ω_S is a constant of the motion.

A lot happened in a very short space here!!!

Heisenberg picture (170). Here, we *define* the H-picture state vector and operator as shown in (24.7) and (24.8). Now the state vector never moves in time, but the operators (which represent variables in your problem like momentum, say) do move in time, not just due to possible explicit motion, but due to inherent motion in this picture, driven by the Hamiltonian. If you simply apply d/dt to (24.8), you get the famous result (24.10) which says how an operator moves in the HS in time! As before, we get the minus sign (this time from the - in the second exponential) and the same commutator as before. Again, state vector stays put, all operators move. However, H does not move. [no explicit-t H yet!]

In the other derivation leading to (24.9), there is a trick involved. You have to ask: why is the first RHS term in (24.6) the same as the first RHS term in (24.9)? You have to think of $\{\partial\Omega_S/\partial t\}$ itself as an operator in the S picture, and you move it to the H picture as you move any other operator. This is what is meant by the line following equation (24.9).

So we now have the very famous equation (24.10) for the Heisenberg picture.

If you look at any scalar product such as $<\alpha|\ \beta>$ or $<\alpha|$ Op $\beta>$, it stays the same as you change pictures (both vectors and operators)! The reason is that the picture changer is a unitary operator $\exp(iHt/\hbar)$. Schiff uses the word "picture" to distinguish from a basis change which changes the "representation". I presume this was standard language before Schiff wrote this book.

Interaction picture (171). Very good. Treat $H = H_o + H'(t)$, nothing small yet. Then move from S to the I picture by using the (24.7) and (24.8) *but* only use H_o (no explicit time dependence). This is shown in (24.12). After some math, you end up with (24.13) and (24.14) which say this:

"In the Interaction picture, the motion of the state vectors is driven only by the H' term of the Hamiltonian, and the motion of the operators is driven only by the H_o term of the Hamiltonian. "

Now, suppose $H' << H_o$ in some sense. Then you are perturbing the states of the H_o system, and you can then use "perturbation theory" to solve problems. This method underlies everything I have ever done in particle physics! It underlies all physical calculations. Yes, we usually write the Lagrangian instead, but I am sure it is exactly the same idea. QED is based on this. The notion of atomic electronic transitions induced by a perturbing EM field is based on this idea. It is extremely important.

Energy Representation (173). We can regard our former energy states $|k>$ as being $|k_S(t=0)>$. The time dependent state $|k_S(t)>$ moves as shown in (24.15), familiar to me, the energy phasor. Now, consider:

$$<k_S(t)\ |\Omega_S|\ k'_S(t)> = \exp[i(E_k - E_{k'})t/\hbar]\ <k|\Omega_S|k'>$$

So if Ω_S itself has no explicit time dependence, this shows that off-diagonal matrix elements of operators in the energy rep have phasors with the energy difference in them. This at least suggests to us the idea of a photon inducing a transition between two states, but Schiff's comment is a little vague at this point. The point is that the energy difference is what appears here! The diagonal matrix elements don't have any time dependence!

Classical vs Quantum Theory (173). Well now comes the big payoff. Schiff reviews classical mechanics from the variation idea to the Lagrange equations of motion. One then defines the Hamiltonian as shown and we get the Hamiltonian equations of motion. [question of whether you should cap L and H ? Goldstein puts caps, Schiff does not.] You can easily derive dF/dt as shown in page middle, and the Poisson Bracket magically appears! The minus sign comes from the minus sign in one of the Ham equations. So you end up with (24.22) which shows the behavior of a function F of the phase space variables.

Poisson vs Commutator Brackets (175). If you make the substitution (24.23), then classical mechanics aligns exactly with the Heisenberg picture, although the constant $\hbar$ is not determined by doing this, it could be anything. In classical, the thing F is a function of phase space. In QM, it is an operator. Two points are now made in this section:

(1) if you imagine that $p_x = -i\hbar\ d/dx$, then the commutator $[x,p_x]$ equations all look exactly like the Poisson bracket equations for x and p_x as classical variables.

(2) Poisson brackets have same algebraic properties as commutator brackets.

Goldstein is given as a reference in several places.

Problem 9 on page 186 shows that in the limit $\hbar \rightarrow 0$, the commutator becomes the Poisson bracket, if you assume your operators are functions of phase space, and you assume $[x,p] = i\hbar$. I have not done this

problem, but you have to go figure out things like $[x^n p^m , x^j p^k]$ which would take some time to do. This has a familiar ring to it somehow, from the very ancient past.

Quantization of a Classical System (176). I guess this is what "first quantization" refers to. Take a classical system, get equations into Poisson Bracket form, then replace with commutator as shown. Also, assume phase space p and q have the usual commutator rules. Then you have arrived at the quantum mechanics Heisenberg picture!

In doing this, there will be some ambiguities involving ordering [recall normal ordering from days of old, but I think that is on 2nd quantization] . Use the average. There will be several QM theories that have the same classical limit as $\hbar \to 0$, we pick the simplest. This is why spin does not appear in the basic EM model we are about to do.

Motion of a particle in an EM field (177). The classical Lagrangian for a non-relativistic particle in a field is this: [we just assume this for right now, see few paragraphs below for the $p_\mu A^\mu$ part.]

$$L(r,v) = 1/2\ mv^2 + q/c\ \mathbf{v}\bullet\mathbf{A}(\mathbf{r},t) - qV(\mathbf{r},t) = p^2/2m + q\ [\mathbf{p}\bullet\mathbf{A}/c - V\ ] = p^2/2m + (q/mc)\ p_\mu A^\mu$$

where **A** and V are the magnetic and electric potentials. What does the Lagrange equation say about this?

$$d/dt\ (\partial L/\partial v_i) = \partial L/\partial x_;$$

If you do the algebra, you quickly arrive at this point: [using $d/dt(A_i) = \partial/\partial t A_i + v_j\, \partial_j A_i$, sum on j]

$$m\dot{v}_i = -\ q\ \partial_i V + (q/c)\ \{\ v_j\ [\ \partial_i A_j - \partial_j A_i\ ]\ \}$$ implied sum on j

The quantity in {..} is equal to $[\ v \times (\nabla \times A)\ ]_i$ but I have no standard vector identity which proves this fact just because there is no clean way to write it! Here is a proof:

$$[\ v \times (\nabla \times A)\ ]_i = \varepsilon_{ijk} v_j\ [\ \varepsilon_{k\ell m}\ \partial_\ell A_m] = v_j\ (\varepsilon_{kij}\ \varepsilon_{k\ell m})\partial_\ell A_m$$

$$= v_j\ [\ \delta_{i\ell}\ \delta_{jm} - \delta_{im}\delta_{j\ell}]\ \partial_\ell A_m = v_j\ [\ \partial_i A_j - \partial_j A_i] \qquad \text{QED}$$

Therefore our assumed Lagrangian has given us

$$m\dot{v}_i = -\ q\ \partial_i V + (q/c)\ [\ v \times (\nabla \times A)\ ]_i = -\ q\ \partial_i V + (q/c)\ [v \times B]_i$$

or

$$m\dot{\mathbf{v}} = -q\ \nabla V + (q/c)\ \mathbf{v} \times \mathbf{B}$$

which is the correct EM force on a particle of charge q. Since this is the known correct equation of motion, our starting Lagrangian must be one that is acceptable for the job. (ie, this was a proof of that L).

Now here is another way to arrive at this conclusion: [$p_0 = E/c \approx mc^2/c = mc$]

$$p_\mu A^\mu = \mathbf{p}\bullet\mathbf{A} - p_o V = m\mathbf{v}\bullet\mathbf{A} - mcV$$ non-relativistic p_0 , setting c = 1

$$= mc\ [\ \mathbf{p}\bullet\mathbf{A}/\mathbf{c} - V\ ]$$

So it must be the quantity **p•A** - V which appears together. See Jackson page 407 for a similar theme.

One you assume the above for a Lagrangian, you quickly arrive at the Hamiltonian Schiff gives. Here is a web derivation of this last step. Notice that the "generalized momentum" is **p** = m**v** + (q/c)**A** and is not just **p** = m**v** because that is what the definition of p says in the L/H formalism. The algebra is not at all obvious, you have to actually do it, but the answer is correct

---

A good illustration of Hamiltonian mechanics is given by the Hamiltonian of a charged particle in an electromagnetic field. In Cartesian coordinates (i.e. *qi* = *xi*), the Lagrangian of a non-relativistic classical particle in an electromagnetic field is (in SI Units):

$$L = \sum_i \tfrac{1}{2} m \dot{x}_i^2 + \sum_i e \dot{x}_i A_i - e\phi,$$

where e is the electric charge of the particle (not necessarily the electron charge), φ is the electric scalar potential, and the *Ai* are the components of the magnetic vector potential (these may be modified through a gauge tranformations).

The generalized momenta may be derived by:

$$p_j = \frac{\partial L}{\partial \dot{x}_j} = m\dot{x}_j + eA_j.$$

Rearranging, we may express the velocities in terms of the momenta, as:

$$\dot{x}_j = \frac{p_j - eA_j}{m}.$$

If we substitute the definition of the momenta, and the definitions of the velocities in terms of the momenta, into the definition of the Hamiltonian given above, and then simplify and rearrange, we get:

$$H = \sum_i \dot{x}_i p_i - L = \sum_i \frac{(p_i - eA_i)^2}{2m} + e\phi.$$

This equation is used frequently in quantum mechanics.

So we end up with exactly equation (24.29) for the Hamiltonian. The effect of the vector field **A** is completely incorporated by adjusting **p** as shown.

Comments: It is not easy to find L and H for a non-relativistic classical charged particle in an EM field! None of my books have it on a quick tour. An E&M book like B&B writes the vxB force and all that stuff, but has no reason to talk about a Lagrangian or a Hamiltonian. Same for Portis and my other E&M books and even Jackson. A QM book or modern physics book is not interested in this topic. Goldstein does not talk about EM fields. [wrong, see p 21 and my notes] Of course when you do Jackson relativistic or B&D, you are going to see the full result which I don't want to digress into right now.

Evaluation of commutator brackets (177). Here Schiff is just doing some pure math to arrive at some commutator results he will no doubt call upon later, as is his habit. The result (24.33) is obvious if you think of $\mathbf{p} = -i\hbar\nabla$ and apply to some function g(r). I did not do the details here.

Velocity and acceleration of a charged particle (178). In (35) Schiff writes out our H, and carefully maintains the correct ordering of **p** and **A** from the squared quantity. He then replaces just one of these p's with gradient. Equation (36) follows at once form the way the canonical **p** was defined, see web clip above (and we ignore all the factors of c). We then arrive at the last equation on page 178. He is now using the Heisenberg picture equation of motion (24.10) to replaced the time derivatives of operators. The operator p_x has no explicit time dependence so you just get the commutator, whereas A does have explicit time dependence. Now you have to compute these horrible commutators and when all the clouds settle, you end up with (24.38) where ordering is maintained. He claims that in QM the velocity and H (ie, magnetic) field operator won't commute in general (not obvious to me but OK), but by fudging you ignore this fact and you end up with the correct equation of motion for a classical particle in an EM field.

I think he is claiming that (24.38) as shown is the correct QM equation where everything is a HS operator including the fields.

Eq (24.39) is the time dependent SE using H from (24.35).

Comment on the above: Starting with the Hamiltonian with the EM field added in the usual way, we think of everything as being an operator, including the EM potentials and fields (something not usually done I think). If we then apply the Heisenberg Picture equations for operators A and p, we end up with an "equation of motion" that is the Lorentz Force law, BUT, everything is a Hilbert Space operator. Ordering is significant. In the classical limit of the result, ordering does not matter.

Virial Theorem (180). Something I don't care about right now, so skip. This theorem in EM says that the kinetic energy is half the potential energy in a 1/r potential, but it has big significance in many applications. [Note added: I have since read all of Goldstein, and he does the virial theorem on page 180 using the famous Virial of Clausius called G. This section is must a mirror image of Goldstein's classical result, and seems to me to just be a restatement of Ehrenfest or the correspondence principle. Whenever you do a time derivative on some <X>, it is good to use the Heisenberg picture (as he silently does here) so you then don't have to think about time dependence of the state.

25. Matrix theory of a harmonic oscillator (180). So here is the simplest non-trivial system you could study in "matrix quantum mechanics", so let's read this section. We start with our Hamiltonian in the usual form, and our p,x commutator as shown.

Energy Representation (181). Equations (25.4) are just calculated from our knowledge of H. But then using the energy representation states we get the two equations in (25.6) trivially (we take general diagonal or non-diagonal elements) and we end up with (25.7) which really says this if you follow through all his words:

Either the matrix element of p (and also x) between states ℓ and k is 0, OR
the energy difference between these states is $\pm\hbar\omega$.

Now I know that states that are 2 or more apart on the ladder will have the first true, and adjacent states will have the second true, but that does not seem to tell me in any obvious way that we have $(n+1/2)\hbar\omega$ as

our spectrum as his words imply, if I did not already know about the ladder. [For example, perhaps the spectrum consists of only two states where each has a huge degeneracy and the spacing between these two states is $\hbar\omega$. I don't think he claims that $(n+1/2)\hbar\omega$ is shown yet, it is just consistent.

Raising and lowering operators (182). If the first factor shown here vanishes, then the second factor need not vanish and this can only happen if the shown lowering operator changes $|\ell\rangle$ to $|k\rangle$. [but the logic seems weak, why can't both factors in equation A vanish in this case?] At some point he argues that the lowering operator has to hit 0, otherwise you get illegal negative energy states. If we raise and then lower the ground state $|0\rangle$, we learn that it has energy $1/2\ \hbar\omega$. We can then generate the other states using the raising operator and get the energy eigenvalues to be $E_n = (n+1/2)\hbar\omega$.

By normalizing the raising and lowering operators, he defines a and $a^\dagger$. We then get the usual commutator rule that $[a, a^\dagger] = 1$ and we can write H as $H = (a^\dagger a + 1/2)\hbar\omega$. Schiff then comments on the future section of the book where $a^\dagger a$ will be the number operator saying the number of quanta in a field, and will therefore be called a creation operator. I recall being fairly excited about this idea in 1972.

I think I could have done this section better than Schiff has done it. Saxon expends pages 131-143 of his book doing perhaps a clearer version of this approach. Since we can talk about matrices in the energy basis of operators like $a^\dagger$, I guess this subject is appropriate for this "matrix QM" chapter of Schiff.

Matrices for a, x and p (183). Without much work, he is able to write the matrices for a and $a^\dagger$ as shown. Each one has numbers only on the first off-diagonal. Our basis $|n\rangle$ here, our representation, are the energy eigenstates.

Coordinate representation (184). First, he gets the wavefunction for the ground state, again, with very little work. He then starts applying raising operators and ends up with the nice Rodriguez form of the Hermites. The answers are shown in (25.16).

So, <u>as promised</u>, Schiff has used "matrix quantum mechanics" to obtain both the energy values and the wavefunctions for a harmonic oscillator. This same problem was treated in Section 13 in the traditional manner.

Summary of Chapter 6: And so ends this *very nice* 37-page Chapter of Schiff where very many things were presented: matrix algebra, the Hilbert Space, the state vector, bra-ket notation, the notion of representations other than the coordinate representation, the various "pictures", including the interaction picture, the connection to classical theory and Poisson Brackets (non-quantum, that is to say), an application of particle + EM field just showing what L and H are and how these give the usual equations, and finally a complete solution of the 1D harmonic oscillator for energies and eigenfunctions.

I presume this is all mentioned somewhere in Messiah and maybe some other books I have, but this is the most concentrated quick dose I think I have.

Test Question #1: The transformations like W are said to be unitary. But when presented in bra-ket form such as $W_{m\mu} = \langle m|\mu\rangle$, the properties of the scalar product make it seem that W is hermitian:

$$W_{m\mu} = \langle m|\mu\rangle = \langle \mu\ |m\rangle^* = W_{\mu m}{}^* = W^\dagger{}_{m\mu} \qquad \Rightarrow W = W^\dagger$$

Are these transformations hermitian as well as unitary? Page 164 explicitly says this:

$$w_{k\mu} = \langle k|\mu\rangle = \langle \mu\ |k\rangle^* \qquad \text{to which I then add} \quad = w_{\mu k}{}^* = w^\dagger{}_{k\mu}$$

Comment: If a matrix is hermitian, you say $A = A^\dagger$. This says $(A^\dagger)_{ab} = (A)_{ab}$ or $(A^*)_{ba} = (A)_{ab}$. Schiff on page 151 does point out that "only square matrices can be Hermitian." When we write $(A^*)_{ba} = (A)_{ab}$ I agree that A has to be square at least if finite-dimensional. Unclear to me if infinite dimensional.

Resolution: Messiah on page 288 of Vol I addresses exactly this question! He would point out that I have an error above in the last equality of this line:

$$W_{m\mu} = \langle m|\mu\rangle = \langle \mu|m\rangle^* = W_{\mu m}^*$$

He argues that $\langle \mu|m\rangle$ is in fact some *other* matrix call it P. Then we have

$$W_{m\mu} = \langle m|\mu\rangle = \langle \mu|m\rangle^* = P_{\mu m}^* = P^\dagger_{m\mu} \qquad \text{so } W = P^\dagger$$

On the bottom of page 288 you see Messiah saying $T = S^\dagger$ which is exactly this point.

Messiah talks all about the three "pictures" above, but he calls them "representations". So this is why Schiff makes his comment about calling them pictures.

This would be a good time to re-read Messiah, but I will resist the temptation and get back to dealing with the secular approximation!