

**Quantum Mechanics****NAME:**

**Homework 3: Formalism:** Homeworks are not handed in or marked. But you get a mark for reporting that you have done them. Once you've reported completion, you may look at the already posted supposedly super-perfect solutions.

**Answer Table for the Multiple-Choice Questions**

	a	b	c	d	e		a	b	c	d	e
1.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	16.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
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007 qmult 00100 1 1 5 easy memory: vector addition

1. The sum of two vectors belonging to a vector space is:
  - a) a scalar.
  - b) another vector, but in a different vector space.
  - c) a generalized cosine.
  - d) the Schwarz inequality.
  - e) another vector in the same vector space.

**SUGGESTED ANSWER:** (e)

**Wrong Answers:**

- b) Exactly wrong.

**Redaction:** Jeffery, 2001jan01

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007 qmult 00200 1 4 4 easy deducto-memory: Schwarz inequality

2. "Let's play *Jeopardy!* For \$100, the answer is:  $|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$ ."

What is \_\_\_\_\_, Alex?

- a) the triangle inequality
- b) the Heisenberg uncertainty principle
- c) Fermat's last theorem
- d) the Schwarz inequality
- e) Schubert's unfinished last symphony

**SUGGESTED ANSWER:** (d)

**Wrong answers:**

- a) Semi-plausible: that's the other simple inequality of vector space linear algebra.
- b) Where's  $\hbar$ ?
- c) Andrew Wiles finally proved this theorem in 1994. See <http://www-groups.dcs.st-andrews.ac.uk/~history/HistTopics/>.
- e) There's some famous unfinished symphony. It may be Schubert's.

**Redaction:** Jeffery, 2001jan01

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007 qmult 00300 1 4 5 easy deducto-memory: Gram-Schmidt procedure

3. Any set of linearly independent vectors can be orthonormalized by the:

- a) Pound-Smith procedure.
- b) Li Po tao.
- c) Sobolev method.
- d) Sobolev-P method.
- e) Gram-Schmidt procedure.

**SUGGESTED ANSWER:** (e)

**Wrong Answers:**

- a) A play on the real answer.
- b) Li Po was 8th century Chinese poet: see <http://www.santafe.edu/~shalizi/Poetry/>.  
Tao can also be a personal name: e.g. Tao Pang my old friend at University of Nevada, Las Vegas.
- c) A radiative transfer method for moving atmospheres.
- d) A variation on the Sobolev method for treating polarized transfer. It's all my own invention.

**Redaction:** Jeffery, 2001jan01

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007 qmult 00400 1 4 4 moderate memory: definition unitary matrix

4. A unitary matrix is defined by the expression:

- a)  $U = U^T$ , where superscript  $T$  means transpose.
- b)  $U = U^\dagger$ .
- c)  $U = U^*$ .
- d)  $U^{-1} = U^\dagger$ .
- e)  $U^{-1} = U^*$ .

**SUGGESTED ANSWER:** (d)

**Wrong Answers:**

- a) Symmetric matrix.

- b) Hermitian matrix.
- c) Real matrix.
- e) Some kind of matrix.

**Redaction:** Jeffery, 2001jan01

007 qmult 00500 2 3 4 moderate math: trivial eigenvalue problem

5. What are the eigenvalues of

$$\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} ?$$

- a) Both are 0.
- b) 0 and 1.
- c) 0 and  $-1$ .
- d) 0 and 2.
- e)  $-i$  and 1.

**SUGGESTED ANSWER:** (d) The eigenvalue equation is

$$0 = (1 - \lambda) - 1 = -2\lambda + \lambda^2$$

which clearly has solutions 0 and 2.

**Wrong Answers:**

- e) As the matrix is Hermitian, it's eigenvalues must be pure real:  $-i$  cannot be an eigenvalue.

**Redaction:** Jeffery, 2001jan01

007 qfull 00090 1 5 0 easy thinking: ordinary vector space

**Extra keywords:** (Gr-77:3.1)

6. Consider ordinary 3-dimensional vectors with complex components specified by a 3-tuple:  $(x, y, z)$ . They constitute a 3-dimensional vector space. Are the following subsets of this vector space vector spaces? If so, what is their dimension? **HINT:** See Gr-435 for all the properties a vector space must have.

- a) The subset of all vectors  $(x, y, 0)$ .
- b) The subset of all vectors  $(x, y, 1)$ .
- c) The subset of all vectors of the form  $(a, a, a)$ , where  $a$  is any complex number.

**SUGGESTED ANSWER:**

- a) It would be pedantic to enumerate the properties. The subset of all vectors  $(x, y, 0)$  is clearly a vector space of dimension 2. The dimensionality is clear since one only needs two basis vectors to construct any member: say  $(1, 0, 0)$  and  $(0, 1, 0)$ .
- b) Nyet: the sum of two members of the subset, e.g.,

$$(x_1, y_1, 1) + (x_2, y_2, 1) = (x_1 + x_2, y_1 + y_2, 2)$$

is not in the subset.

- c) Da—if that is Russian for yes. The subset is, in fact, isomorphic to the set of complex numbers. The only basis vector of the set can be chosen conveniently to be  $(1, 1, 1)$ . With only one basis vector needed the set is 1-dimensional.

**Redaction:** Jeffery, 2001jan01

007 qfull 00100 2 5 0 moderate thinking: vector space, polynomial

**Extra keywords:** (Gr-78:3.2)

7. A vector space is constituted by a set of vectors  $\{|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \dots\}$  and a set of scalars  $\{a, b, c, \dots\}$  (ordinary complex numbers is all that quantum mechanics requires) subject to two operations vector addition and scalar multiplication obeying the certain rules. Note it is the relations between vectors that make them constitute a vector space. What they “are” we leave general. The rules are:

- i) A sum of vectors is a vector:

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle ,$$

where  $|\alpha\rangle$  and  $|\beta\rangle$  are any vectors in the space and  $|\gamma\rangle$  also in the space. Note we have not defined what vector addition consists of. That definition goes beyond the general requirements.

ii) Vector addition is commutative:

$$|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle .$$

iii) Vector addition is associative:

$$(|\alpha\rangle + |\beta\rangle) + |\gamma\rangle = |\alpha\rangle + (|\beta\rangle + |\gamma\rangle) .$$

iv) There is a zero or null vector  $|0\rangle$  such that

$$|\alpha\rangle + |0\rangle = |\alpha\rangle ,$$

v) For every vector  $|\alpha\rangle$  there is an inverse vector  $|\alpha^{-1}\rangle$  such that

$$|\alpha\rangle + |\alpha^{-1}\rangle = |0\rangle .$$

vi) Scalar multiplication of a vector gives a vector:

$$a|\alpha\rangle = |\beta\rangle .$$

vii) Scalar multiplication is distributive on vector addition:

$$a(|\alpha\rangle + |\beta\rangle) = a|\alpha\rangle + a(|\beta\rangle) .$$

viii) Scalar multiplication is distributive on scalar addition:

$$(a + b)|\alpha\rangle = a|\alpha\rangle + b|\alpha\rangle .$$

ix) Scalar multiplication is associative with respect to scalar multiplication:

$$(ab)|\alpha\rangle = a(b|\alpha\rangle) .$$

x) One has

$$0|\alpha\rangle = |0\rangle .$$

xi) Finally, one has

$$1|\alpha\rangle = |\alpha\rangle .$$

**NOTE:** Note that

$$|0\rangle = 0|\alpha\rangle = [1 + (-1)]|\alpha\rangle = |\alpha\rangle + (-1)|\alpha\rangle ,$$

and thus we find that

$$|\alpha^{-1}\rangle = -|\alpha\rangle .$$

So the subtraction of a vector is just the addition of its inverse. This is consistent with all ordinary math.

If any vector in the space can be written as linear combination of a set of linearly independent vectors, that set is called a basis and is said to span the set. The number of vectors in the basis is the dimension of the space. In general there will be infinitely many bases for a space.

Finally the question. Consider the set of polynomials  $\{P(x)\}$  (with complex coefficients) and degree less than  $n$ . For each of the subsets of this set (specified below) answer the following questions: 1) Is the subset a vector space? Inspection usually suffices to answer this question. 2) If not, what property does it lack? 3) If yes, what is the most obvious basis and what is the dimension of the space?

a) The subset that is the whole set.

- b) The subset of even polynomials.
- c) The subset where the highest term has coefficient  $a$  (i.e., the leading coefficient is  $a$ ) and  $a$  is a general complex number, except  $a \neq 0$ .
- d) The subset where  $P(x = g) = 0$  where  $g$  is a general real number. (To be really clear, I mean the subset of polynomials that are equal to zero at the point  $x = g$ .)
- e) The subset where  $P(x = g) = h$  where  $g$  is a general real number and  $h$  is a general complex number, except  $h \neq 0$ .

**SUGGESTED ANSWER:**

- a) By inspection the set has all the requisite properties, and so does constitute a vector space. The set  $\{x^\ell\}$  with  $\ell$  an integer in the range  $[0, n - 1]$  is an obvious basis set for the vector space since the elements are all linearly independent and any polynomial of degree less than  $n$  can be constructed by linear combination from them. From the number of basis vectors we conclude that the dimension of the space is  $n$ .

Note the choice of basis is obvious and convenient, but not unique. For example say we define

$$a_+ = x^1 + x^0$$

and

$$a_- = x^1 - x^0 .$$

We can construct the two lowest degree basis vectors  $x^0$  and  $x^1$  from  $a_+$  and  $a_-$ :

$$x^1 = \frac{1}{2}(a_+ + a_-)$$

and

$$x^0 = \frac{1}{2}(a_+ - a_-) .$$

Therefore we can replace  $x^0$  and  $x^1$  in the basis by  $a_+$  and  $a_-$  to create a new basis. Note also that  $a_+$  and  $a_-$  are in fact independent. Say we tried to set

$$a_- = Ca_+ + \text{linear combination of other basis vectors} ,$$

where  $C$  is some constant to be determined. The other basis vectors have no  $x^0$  or  $x^1$  in them, and so can contribute nothing. Solving for  $C$  we find that  $C$  must equal both 1 and  $-1$ . This is impossible:  $a_+$  and  $a_-$  are thus proven to be linearly independent.

- b) By inspection the set has all the requisite properties, and so does constitute a vector space. The set  $\{x^\ell\}$  with  $\ell$  an even integer in the range  $[0, n - 2]$  if  $n$  is even and  $[0, n - 1]$  if  $n$  is odd is an obvious basis set for the vector space since the elements are all linearly independent and any even polynomial of degree less than  $n$  can be constructed by linear combination from them. The dimension of the space is  $(n - 2)/2 + 1 = n/2$  if  $n$  is even and  $(n - 1)/2 + 1 = (n + 1)/2$  if  $n$  is odd. The fact that there is a  $x^0$  vector in our convenient basis clues us in that there must be those “+1”’s in the expressions for the dimensions—if it wasn’t obvious from the foregoing.
- c) No. The polynomial that is the sum of two elements have leading coefficient  $2a$ , and thus this polynomial is not in the specified subset.
- d) By inspection the set has all the requisite properties, and so does constitute a vector space. The set  $\{(x - g)^\ell\}$  with  $\ell$  an integer in the range  $[1, n - 1]$  is a natural basis set for the vector space since the elements are all linearly independent and any polynomial in the subset of order less than  $n$  can be constructed by linear combination from them. Maybe a demonstration is needed. Say  $P(x)$  is a general element in the subset, then

$$\begin{aligned} P(x) &= \sum_{\ell=0}^{n-1} a_\ell x^\ell = \sum_{\ell=0}^{n-1} a_\ell [(x - g) + g]^\ell \\ &= \sum_{\ell=0}^{n-1} b_\ell (x - g)^\ell = \sum_{\ell=1}^{n-1} b_\ell (x - g)^\ell , \end{aligned}$$

where we have done a rearrangement of terms using the binomial theorem implicitly and where we have recognized that  $b_0 = 0$  since by hypothesis  $P(x)$  is in the subset. Since  $P(x)$  is a general member of the subset,  $\{(x - g)^\ell\}$  is a basis for the subset. The dimension of the space is obviously  $n - 1$ : there is no place for the non-existent  $(x - g)^0$  unit vector.

- e) No. The polynomial that is the sum of two elements when evaluated at  $g$  equals  $2h$ , and thus polynomial is not in the specified subset.

**Redaction:** Jeffery, 2001jan01

007 qfull 00110 2 5 0 moderate thinking: unique expansion in basis

**Extra keywords:** (Gr-78:3.3)

8. Prove that the expansion of a vector in terms of some basis is unique: i.e., the set of expansion coefficients for the vector is unique.

**SUGGESTED ANSWER:**

Say  $|\psi\rangle$  is a general vector of the vector space for which  $\{|\phi_i\rangle\}$  is the basis. Assume that we have two different expansions

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle = \sum_i d_i |\phi_i\rangle ,$$

then

$$0 = \sum_i (c_i - d_i) |\phi_i\rangle .$$

But since the basis vectors all independent by the hypothesis that they are basis vectors, no term  $i$  can be completely eliminated by any combination of the other terms. The only possibility is that  $c_i - d_i = 0$  for all  $i$  or  $c_i = d_i$  for all  $i$ . Thus, our two different expansions must, in fact, be the same. An expansion is unique.

If one would like a more concrete demonstration, assume that  $c_j - d_j \neq 0$  for some  $j$ . Then we can divide the second sum above through by  $c_j - d_j$ , move  $|\phi_j\rangle$  to the other side, and multiply through by  $-1$  to get

$$|\phi_j\rangle = - \sum_{i, \text{ but } i \neq j} \left( \frac{c_i - d_i}{c_j - d_j} \right) |\phi_i\rangle .$$

But now we find  $|\phi_j\rangle$  is a linear combination of the other “basis” vectors. This cannot be if our vectors are independent. We conclude again that  $c_i = d_i$  for all  $i$  and the expansion is unique.

**Redaction:** Jeffery, 2001jan01

007 qfull 00200 3 5 0 tough thinking: Gram-Schmidt orthonormalization

**Extra keywords:** (Gr-79:3.4)

9. Say  $\{|\alpha_i\rangle\}$  is a basis (i.e., a set of linearly independent vectors that span a vector space), but it is not orthonormal. The first step of the Gram-Schmidt orthogonalization procedure is to normalize the (nominally) first vector to create a new first vector for a new orthonormal basis:

$$|\alpha'_1\rangle = \frac{|\alpha_1\rangle}{\|\alpha_1\|} ,$$

where recall that the norm of a vector  $|\alpha\rangle$  is given by

$$\|\alpha\| = \|\alpha_1\| = \sqrt{\langle\alpha|\alpha\rangle} .$$

The second step is create a new second vector that is orthogonal to the new first vector using the old second vector and the new first vector:

$$|\alpha'_2\rangle = \frac{|\alpha_2\rangle - |\alpha'_1\rangle\langle\alpha'_1|\alpha_2\rangle}{\|\alpha_2\rangle - |\alpha'_1\rangle\langle\alpha'_1|\alpha_2\rangle\|} .$$

Note we have subtracted the projection of  $|\alpha_2\rangle$  on  $|\alpha'_1\rangle$  from  $|\alpha_2\rangle$  and normalized.

- a) Write down the general step of the Gram-Schmidt procedure.
- b) Why must an orthonormal set of non-null vectors be a linearly independent.
- c) Is the result of a Gram-Schmidt procedure independent of the order the original vectors are used? **HINT:** Say you first use vector  $|\alpha_a\rangle$  of the old set in the procedure. The first new vector is just  $|\alpha_a\rangle$  normalized: i.e.,  $|\alpha'_a\rangle = |\alpha_a\rangle / \|\alpha_a\|$ . All the other new vectors will be orthogonal to  $|\alpha'_a\rangle$ . But what if you started with  $|\alpha_b\rangle$  which in general is not orthogonal to  $|\alpha_a\rangle$ ?
- d) How many orthonormalized bases can an  $n$  dimensional space have in general? (Ignore the strange  $n = 1$  case.) **HINT:** Can't the Gram-Schmidt procedure be started with any vector at all in the vector space?
- e) What happens in the procedure if the original vector set  $\{|\alpha_i\rangle\}$  does not, in fact, consist of all linearly independent vectors? To understand this case analyze another apparently different case. In this other case you start the Gram-Schmidt procedure with  $n$  original vectors. Along the way the procedure yields null vectors for the new basis. Nothing can be done with the null vectors: they can't be part of a basis or normalized. So you just put those null vectors and the vectors they were meant to replace aside and continue with the procedure. Say you got  $m$  null vectors in the procedure and so ended up with  $n - m$  non-null orthonormalized vectors. Are these  $n - m$  new vectors independent? How many of the old vectors were used in constructing the new  $n - m$  non-null vectors and which old vectors were they? Can all the old vectors be reconstructed from the the new  $n - m$  non-null vectors? Now answer the original question.
- f) If the original set did consist of  $n$  linearly independent vectors, why must the new orthonormal set consist of  $n$  linearly independent vectors? **HINT:** Should be just a corollary of the part (e) answer.
- g) Orthonormalize the 3-space basis consisting of

$$|\alpha_1\rangle = \begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix}, |\alpha_2\rangle = \begin{pmatrix} i \\ 3 \\ 1 \end{pmatrix}, \quad \text{and} \quad |\alpha_3\rangle = \begin{pmatrix} 0 \\ 32 \\ 0 \end{pmatrix}.$$

Input the vectors into the procedure in the reverse of their nominal order: why might a marker insist on this? Note setting kets equal to columns is a lousy notation, but you-all know what I mean. The bras, of course, should be "equated" to the row vectors. **HINT:** Make sure you use the normalized new vectors in the construction procedure.

### SUGGESTED ANSWER:

- a) Behold:

$$|\alpha'_i\rangle = \frac{|\alpha_i\rangle - \sum_{j=1}^{i-1} |\alpha'_j\rangle \langle \alpha'_j | \alpha_i \rangle}{\| |\alpha_i\rangle - \sum_{j=1}^{i-1} |\alpha'_j\rangle \langle \alpha'_j | \alpha_i \rangle \|},$$

where the summation upper limit  $-1$  is interpreted as meaning the whole summation is just a zero.

Just to demonstrate concretely that  $|\alpha'_i\rangle$  is indeed orthogonal to all  $|\alpha'_k\rangle$  with  $k < i$  (i.e., the all already constructed new basis vectors), we evaluate  $\langle \alpha'_k | \alpha'_i \rangle$ :

$$\begin{aligned} \langle \alpha'_k | \alpha'_i \rangle &= \frac{\langle \alpha'_k | \alpha_i \rangle - \sum_{j=1}^{i-1} \langle \alpha'_k | \alpha'_j \rangle \langle \alpha'_j | \alpha_i \rangle}{\| |\alpha_i\rangle - \sum_{j=1}^{i-1} |\alpha'_j\rangle \langle \alpha'_j | \alpha_i \rangle \|} \\ &= \frac{\langle \alpha'_k | \alpha_i \rangle - \sum_{j=1}^{i-1} \delta_{kj} \langle \alpha'_j | \alpha_i \rangle}{\| |\alpha_i\rangle - \sum_{j=1}^{i-1} |\alpha'_j\rangle \langle \alpha'_j | \alpha_i \rangle \|} \\ &= \frac{\langle \alpha'_k | \alpha_i \rangle - \langle \alpha'_k | \alpha_i \rangle}{\| |\alpha_i\rangle - \sum_{j=1}^{i-1} |\alpha'_j\rangle \langle \alpha'_j | \alpha_i \rangle \|} \\ &= 0, \end{aligned}$$

where we have used the fact that the new vectors for  $k < i$  are orthogonal. Pretty clearly  $|\alpha'_i\rangle$  is normalized: it's explicitly so actually. So  $|\alpha'_i\rangle$  is orthonormalized with respect to all the previously constructed new basis vectors.

- b) Quite obviously if the set is orthonormal, none of the set can be expanded in terms of a combination of the others. Since they can't, they are by definition all linearly independent.

To be absolutely concrete assume contrafactually that one of a set of orthonormal vectors is expanded in the others:

$$|\alpha_i\rangle = \sum_{j \neq i} |\alpha_j\rangle .$$

Then take the scalar product with bra  $\langle \alpha_i |$ :

$$\langle \alpha_i | \alpha_i \rangle = 0$$

by orthogonality. But the vectors were non-null by hypothesis, and so our assumption of dependence was wrong.

- c) No. The first vector you input to the procedure yields a normalized version of itself. In general all the other vectors aren't orthogonal to that vector: therefore their counterparts in the new set are not in general just normalized versions of themselves. But you can start the procedure with any of the original vectors you like. Thus you can preserve any one original vector you wish in normalized form, but not in general the others. Thus every starting input vector can in general lead to a different orthonormal set. I think it's intuitively suggested that if you have  $n$  linearly independent original vectors that up to  $n!$  orthonormalized bases can be generated. But the proof is beyond me at this time of night. Hm: it seems obviously true though.
- d) There are infinitely many choices of vector direction in a vector space of dimension  $n \geq 2$ . Any such vector can be used as the starting vector in a Gram-Schmidt procedure. The other  $n - 1$  linear independent original vectors can be obtained from almost any old basis: the  $n - 1$  vectors must be linearly independent of your starting vector of course.
- e) Consider  $n$  vectors in an original set  $\{|\alpha_i\rangle\}$  and carry out the Gram-Schmidt procedure to the end. Along the way  $m$  of the new vectors were null; you just ignored these and the old vectors they were meant to replace. Null vectors can't be normalized or form part of a basis. At the end of the procedure you have a new set of  $n - m$  non-null, orthonormal vectors  $\{|\alpha'_i\rangle\}$ . Since they are orthogonal, they are all linearly independent. Thus the set  $\{|\alpha'_i\rangle\}$  is an orthonormal basis for an  $n - m$  dimensional space.

In constructing the  $n - m$  new vectors you, in fact, used only  $n - m$  of the original vectors: the vectors you used were the  $n - m$  ones that did not give null new vectors.

You can reconstruct the entire original set from the  $n - m$  new vectors. First, every  $|\alpha_i\rangle$  that gave a null vector in the procedure is clearly a linear combination of the newly constructed basis:

$$|\alpha_i\rangle = \sum_{j=1}^{i-1} |\alpha'_j\rangle \langle \alpha'_j | \alpha_i \rangle .$$

Second, every  $|\alpha_i\rangle$  that gave a non-null vector is also a linear combination of the newly constructed basis:

$$|\alpha_i\rangle = \left( \left\| |\alpha_i\rangle - \sum_{j=1}^{i-1} |\alpha'_j\rangle \langle \alpha'_j | \alpha_i \rangle \right\| \right) |\alpha'_i\rangle + \sum_{j=1}^{i-1} |\alpha'_j\rangle \langle \alpha'_j | \alpha_i \rangle .$$

Thus, the original set  $\{|\alpha_i\rangle\}$  is entirely contained in the  $n - m$  space spanned by the new basis.

Since the  $n - m$  new vectors were constructed from  $n - m$  old vectors and the  $n - m$  new vectors can be used to construct any of the  $n$  vectors in the original set, the  $n - m$  old vectors used to construct the new  $n - m$  vectors can be used to construct  $m$  vectors of the original set that gave nulls in the procedure. Thus there were in the original set only  $n - m$  independent vectors and the original set spanned only an  $n - m$  dimensional space. Of course, one doesn't mean that the  $n - m$  old vectors used in the Gram-Schmidt procedure were "the independent" ones and the  $m$  neglected old vectors were "the non-independent" ones. One means some set of  $m$  vectors of the  $n$  old vectors could be constructed from the others and eliminated beforehand from the Gram-Schmidt procedure. Which set of  $m$  old vectors could be chosen in various ways in general depending on the exact nature of the  $n$  old vectors. In the



Gram-Schmidt procedure which  $m$  old vectors get neglected depends in general on the order one chooses to input vectors into the procedure.

Now to answer the original question. If the original set of vectors is not independent then one will get nulls in the Gram-Schmidt procedure. If one doesn't get null vectors, then one constructs independent vectors out of non-independent vectors which is a logical inconsistency. The number of non-null vectors the procedure yields is exactly the number of independent vectors in the original set or (meaning the same thing) is the dimension of the space spanned by the original set. The Gram-Schmidt procedure offers a systematic a way to test for the linear independence of a set of vectors. Every null new vector means one more of the original vectors was not linearly independent.

- f) From the part (e) answer, it follows that if all the original vectors were linearly independent, then no no null vectors are generated in the Gram-Schmidt procedure. Thus the procedure generates  $n$  new vectors given  $n$  old linearly independent vectors. The  $n$  new vectors are clearly linearly independent since they are orthogonal: see the part (b) answer. Thus if the original set consisted of  $n$  linearly independent vectors, the new set must too.
- g) I think inputting the vectors in the reverse of the nominal order gives the simplest result. I insist the student's do so, so that everyone should get the same orthonormalized set if all goes well. Recall from the part (c) answer that the orthonormalized set does depend on the order the original vectors are used in the procedure. Behold:

$$\begin{aligned}
 |\alpha'_3\rangle &= \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\
 |\alpha'_2\rangle &= \frac{\begin{pmatrix} i \\ 3 \\ 1 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \left[ (0, 1, 0) \cdot \begin{pmatrix} i \\ 3 \\ 1 \end{pmatrix} \right]}{\sqrt{\dots}} \\
 &= \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} \\
 |\alpha'_3\rangle &= \frac{\begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \left[ (0, 1, 0) \cdot \begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix} \right] - \frac{1}{2} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} \left[ (-i, 0, 1) \cdot \begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix} \right]}{\sqrt{\dots}} \\
 &= \frac{\begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} (-i+1+i)}{\sqrt{\dots}} \\
 &= \frac{\begin{pmatrix} 1+i \\ 0 \\ i \end{pmatrix} - \frac{1}{2} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix}}{\sqrt{\dots}} \\
 &= \sqrt{\frac{2}{5}} \begin{pmatrix} 1+\frac{i}{2} \\ 0 \\ i-\frac{1}{2} \end{pmatrix}.
 \end{aligned}$$

**Redaction:** Jeffery, 2001jan01

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007 qfull 00300 2 3 0 moderate math: prove the Schwarz inequality

**Extra keywords:** (Gr-80:3.5)

10. As Andy Rooney says (or used to say if this problem has reached the stage where only old fogies remember that king of the old fogies) don't you just hate magic proofs where you start from some

unmotivated expression and do a number of unmotivated steps to arrive at a result that you could never have been guessed from the way you were going about getting it. Well sans too many absurd steps, let us see if we can prove the Schwarz inequality

$$|\langle \alpha | \beta \rangle|^2 \leq \langle \alpha | \alpha \rangle \langle \beta | \beta \rangle$$

for general vectors  $|\alpha\rangle$  and  $|\beta\rangle$ . Note the equality only holds in two cases. First when  $|\beta\rangle = a|\alpha\rangle$ , where  $a$  is some complex constant. Second, when either or both of  $|\alpha\rangle$  and  $|\beta\rangle$  are null vectors: in this case, one has zero equals zero.

**NOTE:** A few facts to remember about general vectors and inner products. Say  $|\alpha\rangle$  and  $|\beta\rangle$  are general vectors. By the definition of the inner product, we have that  $\langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle^*$ . This implies that  $\langle \alpha | \alpha \rangle$  is pure real. If  $c$  is a general complex number, then the inner product of  $|\alpha\rangle$  and  $c|\beta\rangle$  is  $\langle \alpha | c|\beta \rangle = c\langle \alpha | \beta \rangle$ . Next we note that that another inner-product property is that  $\langle \alpha | \alpha \rangle \geq 0$  and the equality only holds if  $|\alpha\rangle$  is the null vector. The norm of  $|\alpha\rangle$  is  $\|\alpha\| = \sqrt{\langle \alpha | \alpha \rangle}$  and  $|\alpha\rangle$  can be normalized if it is not null: i.e., for  $|\alpha\rangle$  not null, the normalized version is  $|\hat{\alpha}\rangle = |\alpha\rangle / \|\alpha\|$ .

- a) In doing the proof of the Schwarz inequality, it is convenient to have the result that the bra corresponding to  $c|\beta\rangle$  (where  $|\beta\rangle$  is a general vector and  $c$  is a general complex number) is  $\langle \beta | c^*$ . Prove this correspondance. **HINT:** Consider general vector  $|\alpha\rangle$  and the inner product

$$\langle \alpha | c|\beta \rangle$$

and work your way by valid steps to

$$\langle \beta | c^* | \alpha \rangle^*$$

and that completes the proof since

$$\langle \alpha | \gamma \rangle = \langle \gamma | \alpha \rangle^*$$

for general vectors  $|\alpha\rangle$  and  $|\gamma\rangle$ .

- b) The next thing to do is to figure out what the Schwarz inequality is saying about vectors including those 3-dimensional things we have always called vectors. Let us restrict the generality of  $|\alpha\rangle$  by demanding it not be a null vector for which the Schwarz inequality is already proven. Since  $|\alpha\rangle$  is not null, it can be normalized. Let  $|\hat{\alpha}\rangle = |\alpha\rangle / \|\alpha\|$  be the normalized version of  $|\alpha\rangle$ . Divide the Schwarz inequality by  $\|\alpha\|^2$ . Now note that the component of  $|\beta\rangle$  along the  $|\hat{\alpha}\rangle$  direction is

$$|\beta_{\parallel}\rangle = |\hat{\alpha}\rangle \langle \hat{\alpha} | \beta \rangle .$$

Evaluate  $\langle \beta_{\parallel} | \beta_{\parallel} \rangle$ . Now what is the Schwarz inequality telling us.

- c) The vector component of  $|\beta\rangle$  that is orthogonal to  $|\hat{\alpha}\rangle$  (and therefore  $|\beta_{\parallel}\rangle$ ) is

$$|\beta_{\perp}\rangle = |\beta\rangle - |\beta_{\parallel}\rangle .$$

Prove this and then prove the Schwarz inequality itself (for  $|\alpha\rangle$  not null) by evaluating  $\langle \beta | \beta \rangle$  expanded in components. What if  $|\alpha\rangle$  is a null vector?

### SUGGESTED ANSWER:

- a) Behold:

$$\langle \alpha | c|\beta \rangle = c\langle \alpha | \beta \rangle = c\langle \beta | \alpha \rangle^* = (c^* \langle \beta | \alpha \rangle)^* = \langle \beta | c^* | \alpha \rangle^* .$$

Since  $|\alpha\rangle$ ,  $|\beta\rangle$ , and  $c$  are general, we find that bra corresponding to general  $c|\beta\rangle$  is  $\langle \beta | c^*$ .

- b) Well doing the suggested division we get

$$|\langle \hat{\alpha} | \beta \rangle|^2 \leq \langle \beta | \beta \rangle .$$

Now we find

$$\langle \beta_{\parallel} | \beta_{\parallel} \rangle = \langle \beta | \hat{\alpha} \rangle \langle \hat{\alpha} | \hat{\alpha} \rangle \langle \hat{\alpha} | \beta \rangle = \langle \beta | \hat{\alpha} \rangle \langle \hat{\alpha} | \beta \rangle = |\langle \hat{\alpha} | \beta \rangle|^2 ,$$

where we have used the part (a) result and the fact that  $\langle \hat{\alpha} | \hat{\alpha} \rangle = 1$ . We see that the left-hand side of the inequality is the magnitude squared of  $|\beta_{\parallel}\rangle$  and the right-hand side is the

magnitude squared of  $|\beta\rangle$ . Now it is clear. The Schwarz inequality just means that magnitude of the component of a vector along some axis is less than or equal to the magnitude of the vector itself.

The equality holds if  $|\beta\rangle$  is aligned with the axis defined by  $|\hat{\alpha}\rangle$ . In this case,

$$|\beta\rangle = a|\hat{\alpha}\rangle ,$$

where  $a$  is some constant, and

$$|\beta_{\parallel}\rangle = a|\hat{\alpha}\rangle\langle\hat{\alpha}|\hat{\alpha}\rangle = a|\hat{\alpha}\rangle = |\beta\rangle .$$

So  $|\beta_{\parallel}\rangle$  is  $|\beta\rangle$  in this case. This is just what the question preamble preambled.

There are contexts in which the Schwarz inequality is used for some purpose not clearly connected to the meaning found above. Most importantly in quantum mechanics, the Schwarz inequality is used in its ordinary form in proving the generalized uncertainty principle (Gr-110).

c) Behold:

$$\langle\hat{\alpha}|\beta_{\perp}\rangle = \langle\hat{\alpha}|\beta\rangle - \langle\hat{\alpha}|\beta_{\parallel}\rangle = \langle\hat{\alpha}|\beta\rangle - \langle\hat{\alpha}|\hat{\alpha}\rangle\langle\hat{\alpha}|\beta\rangle = \langle\hat{\alpha}|\beta\rangle - \langle\hat{\alpha}|\beta\rangle = 0 ,$$

where we have used the normalization of  $|\hat{\alpha}\rangle$ . Since  $|\beta_{\parallel}\rangle = |\hat{\alpha}\rangle\langle\hat{\alpha}|\beta\rangle$  (i.e.,  $|\beta_{\parallel}\rangle$  is parallel to  $|\hat{\alpha}\rangle$ ), we have that  $|\beta_{\perp}\rangle$  is orthogonal to  $|\beta_{\parallel}\rangle$  too.

Now

$$|\beta\rangle = |\beta_{\parallel}\rangle + |\beta_{\perp}\rangle ,$$

and so

$$\begin{aligned} \langle\beta|\beta\rangle &= \langle\beta_{\parallel}|\beta_{\parallel}\rangle + \langle\beta_{\parallel}|\beta_{\perp}\rangle + \langle\beta_{\perp}|\beta_{\parallel}\rangle + \langle\beta_{\perp}|\beta_{\perp}\rangle \\ &= \langle\beta_{\parallel}|\beta_{\parallel}\rangle + \langle\beta_{\perp}|\beta_{\perp}\rangle , \end{aligned}$$

where we have used orthogonality of  $|\beta_{\perp}\rangle$  and  $|\beta_{\parallel}\rangle$ . By an inner-product property, we know that

$$\langle\beta_{\parallel}|\beta_{\parallel}\rangle \geq 0 \quad \text{and} \quad \langle\beta_{\perp}|\beta_{\perp}\rangle \geq 0 .$$

Thus, we have

$$\langle\beta_{\parallel}|\beta_{\parallel}\rangle = |\langle\hat{\alpha}|\beta\rangle|^2 \leq \langle\beta|\beta\rangle .$$

The last expression is equivalent to the Schwarz inequality for  $|\alpha\rangle$  not null as we saw in the part (a) answer. So we have proven the Schwarz inequality for the case that  $|\alpha\rangle$  is not a null vector.

If  $|\alpha\rangle$  is a null vector, then both sides of the Schwarz inequality are zero and the inequality holds in its equality case. This is just what the question preamble preambled.

I have to say that WA-513–514's proof of the Schwarz inequality seems unnecessarily obscure since it hides the meaning of Schwarz inequality. It also deters people from finding the above proof which seems the straightforward one to me and is based on the meaning of the Schwarz inequality.

**Redaction:** Jeffery, 2001jan01

007 qfull 00310 1 3 0 easy math: find a generalized angle

**Extra keywords:** (Gr-80:3.6)

11. The general inner-product vector space definition of generalized angle according to Gr-440 is

$$\cos\theta_{\text{gen}} = \frac{|\langle\alpha|\beta\rangle|}{\sqrt{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle}} ,$$

where  $|\alpha\rangle$  and  $|\beta\rangle$  are general non-zero vectors.

a) Is this definition completely consistent with the ordinary definition of an angle from the ordinary vector dot product? Why or why not?

b) Find the generalized angle between vectors

$$|\alpha\rangle = \begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix} \quad \text{and} \quad |\beta\rangle = \begin{pmatrix} 4-i \\ 0 \\ 2-2i \end{pmatrix} .$$

**SUGGESTED ANSWER:**

a) Well no the definition is not completely consistent. Say  $\vec{a}$  and  $\vec{b}$  are ordinary vectors with magnitudes  $a$  and  $b$ , respectively. If you put them in the generalized angle formula you get

$$\cos \theta_{\text{gen}} = \frac{|\vec{a} \cdot \vec{b}|}{ab} .$$

But the ordinary vector dot product formula is

$$\cos \theta = \frac{\vec{a} \cdot \vec{b}}{ab} .$$

Thus

$$\cos \theta_{\text{gen}} = |\cos \theta| = \begin{cases} \cos \theta , & \text{for } \cos \theta \geq 0; \\ -\cos \theta = \cos(\pi - \theta) , & \text{for } \cos \theta \leq 0. \end{cases}$$

Thus for  $\theta \in [0, \pi/2]$ , we get  $\theta_{\text{gen}} = \theta$  and for  $\theta \in [\pi/2, \pi]$ ,  $\theta_{\text{gen}} = \pi - \theta$ .

b) Well

$$\begin{aligned} \langle \alpha | \alpha \rangle &= 4 , \\ \langle \beta | \beta \rangle &= 25 , \end{aligned}$$

and

$$\langle \alpha | \beta \rangle = (1-i \quad 1 \quad -i) \begin{pmatrix} 4-i \\ 0 \\ 2-2i \end{pmatrix} = 3 - 5i + 0 - 2i - 2 = 1 - 7i .$$

Thus the cosine of the generalized angle is

$$\cos \theta_{\text{gen}} = \frac{\sqrt{1+49}}{2 \times 5} = \frac{1}{5\sqrt{2}} .$$

The corresponding angle is  $\theta_{\text{gen}} = \pi/4 = 45^\circ$ .

**Redaction:** Jeffery, 2001jan01

007 qfull 00400 1 3 0 easy math: prove triangle inequality

**Extra keywords:** (Gr-80:3.7)

12. Prove the triangle inequality:

$$\|(|\alpha\rangle + |\beta\rangle)\| \leq \|\alpha\| + \|\beta\| .$$

**HINT:** Start with  $\|(|\alpha\rangle + |\beta\rangle)\|^2$ , expand, and use reality and the Schwarz inequality

$$|\langle \alpha | \beta \rangle|^2 \leq \langle \alpha | \alpha \rangle \langle \beta | \beta \rangle = \|\alpha\|^2 \times \|\beta\|^2 .$$

**SUGGESTED ANSWER:**

Behold:

$$\begin{aligned} \|(|\alpha\rangle + |\beta\rangle)\|^2 &= \langle \alpha | \alpha \rangle + \langle \beta | \beta \rangle + \langle \alpha | \beta \rangle + \langle \beta | \alpha \rangle \\ &= \langle \alpha | \alpha \rangle + \langle \beta | \beta \rangle + 2\text{Re}[\langle \alpha | \beta \rangle] \\ &\leq \langle \alpha | \alpha \rangle + \langle \beta | \beta \rangle + 2|\langle \alpha | \beta \rangle| \\ &\leq \langle \alpha | \alpha \rangle + \langle \beta | \beta \rangle + 2\|\alpha\| \times \|\beta\| \\ &= \|\alpha\|^2 + \|\beta\|^2 + 2\|\alpha\| \times \|\beta\| \\ &= (\|\alpha\| + \|\beta\|)^2 , \end{aligned}$$

where we have used the Schwarz inequality to get the 4th line. The triangle inequality follows at once:

$$|(|\alpha\rangle + |\beta\rangle)| \leq \|\alpha\| + \|\beta\| .$$

Interpreting the triangle in terms of ordinary vectors, it means that the sum of the magnitudes of the two vectors is always greater than or equal to the magnitude of the vector sum. The equality only holds if the vectors are parallel and not antiparallel. The Schwarz inequality interpreted in terms of ordinary vectors is that the magnitude of a component of a vector along an axis is always less than or equal to the magnitude of the vector. The equality only holds when the vector is aligned with the axis. One can see the situation by dividing the Schwarz inequality by one vector magnitude in order to create a unit vector for an axis: e.g.,

$$|\langle \hat{\alpha} | \beta \rangle|^2 \leq \langle \beta | \beta \rangle .$$

**Redaction:** Jeffery, 2001jan01

007 qfull 00500 3 3 0 tough math: simple matrix identities

**Extra keywords:** (Gr-87:3.12)

13. Prove the following matrix identities:

- a)  $(AB)^T = B^T A^T$ , where superscript “T” means transpose.
- b)  $(AB)^\dagger = B^\dagger A^\dagger$ , where superscript  $\dagger$  means Hermitian conjugate.
- c)  $(AB)^{-1} = B^{-1} A^{-1}$ .
- d)  $(UV)^{-1} = (UV)^\dagger$  (i.e.,  $UV$  is unitary) given that  $U$  and  $V$  are unitary. In other words, prove the product of unitary matrices is unitary.
- e)  $(AB)^\dagger = AB$  (i.e.,  $AB$  is Hermitian) given that  $A$  and  $B$  are commuting Hermitian matrices. Does the converse hold: i.e., does  $(AB)^\dagger = AB$  imply  $A$  and  $B$  are commuting Hermitian matrices? **HINTS:** Find a trivial counterexample. Try  $B = A^{-1}$ .
- f)  $(A + B)^\dagger = A + B$  (i.e.,  $A + B$  is Hermitian) given that  $A$  and  $B$  are Hermitian. Does the converse hold? **HINT:** Find a trivial counterexample to the converse.
- g)  $(U + V)^\dagger = (U + V)^{-1}$  (i.e.,  $U + V$  is unitary) given that  $U$  and  $V$  are unitary—that is, prove this relation if it’s indeed true—if it’s not true, prove that it’s not true. **HINT:** Find a simple counterexample: e.g., two  $2 \times 2$  unit matrices.

**SUGGESTED ANSWER:**

a) Behold:

$$[(AB)^T]_{ij} = (AB)_{ji} = A_{jk} B_{ki} = B_{ki} A_{jk} = B_{ik}^T A_{kj}^T = (B^T A^T)_{ij} ,$$

where we have used the Einstein rule of summation on repeated indices. Since the matrix element is general this completes the proof.

b) Recall that to complex conjugate a matrix is to change its elements to their complex conjugates. Note that

$$[(AB)_{ij}]^* = (A_{ik} B_{kj})^* = A_{ik}^* B_{kj}^* ,$$

and so  $(AB)^* = A^* B^*$ . Thus, complex conjugating the part (a) identity gives

$$(AB)^{T*} = B^{T*} A^{T*}$$

or

$$(AB)^\dagger = B^\dagger A^\dagger ,$$

which completes the proof. Note that the effect of the complex conjugation and transpose operations is independent of order.

c) Note

$$(AB)^{-1}(AB) = \mathbf{1}$$

where  $\mathbf{1}$  is the unit matrix. Thus

$$(AB)^{-1}A = B^{-1} \quad \text{and} \quad (AB)^{-1} = B^{-1}A^{-1},$$

which completes the proof.

d) Behold:

$$(UV)^{-1} = V^{-1}U^{-1} = V^\dagger U^\dagger = (UV)^\dagger.$$

e) Behold:

$$AB = BA = B^\dagger A^\dagger = (AB)^\dagger,$$

and so  $AB$  is Hermitian given that  $A$  and  $B$  are commuting Hermitian operators.

Is the converse of the above result true? Say we are given that  $AB$  is Hermitian. Then we know

$$AB = (AB)^\dagger = B^\dagger A^\dagger,$$

but I don't think that we can make any further very general statements about  $A$  and  $B$ . The converse probably doesn't hold, but to be sure one would have to find a counterexample. Well how about the trivial counterexample where  $B = A^{-1}$ . We know that  $AA^{-1} = \mathbf{1}$ , where  $\mathbf{1}$ , the unit matrix, is trivially Hermitian. But any nonsingular matrix  $A$  has an inverse, and they aren't all Hermitian. For example

$$A = \begin{pmatrix} 0 & 2 \\ 1 & 0 \end{pmatrix}$$

is not Hermitian and has an inverse:

$$\begin{pmatrix} 0 & 2 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ \frac{1}{2} & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The converse is false.

f) Behold:

$$(A + B)^\dagger = A^\dagger + B^\dagger = A + B.$$

So the "forverse" is true. The converse is not true: i.e.,  $(A + B)^\dagger = A + B$  does not imply  $A$  and  $B$  are Hermitian. For example

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

are not Hermitian, but their sum clearly is.

g) The suggested counterexample is too trivial we all agree. Instead consider the following matrices which are both Hermitian and their own inverses, and hence are unitary:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Their sum

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

is its own Hermitian conjugate, but this Hermitian conjugate is not the inverse:

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}$$

Thus the sum of unitary matrices is not in general unitary.

**Redaction:** Jeffery, 2001jan01

14. There are 4 simple operations that can be done to a matrix: inverting,  $(-1)$ , complex conjugating  $(*)$ , transposing  $(T)$ , and Hermitian conjugating  $(\dagger)$ . Prove that all these operations mutually commute. Do this systematically: there are

$$\binom{4}{2} = \frac{4!}{2!(4-2)!} = 6$$

combinations of the 2 operations. We assume the matrices have inverses for the proofs involving them.

**SUGGESTED ANSWER:** We will do the proofs in nearly wordless sequences for brevity and clarity.

- i) For  $-1$  and  $*$ :

$$\begin{aligned} \mathbf{1} &= AA^{-1}, \\ \mathbf{1} &= (AA^{-1})^*, \\ \mathbf{1} &= A^*(A^{-1})^*, \\ (A^*)^{-1} &= (A^{-1})^*. \end{aligned}$$

Note  $\mathbf{1}$  is the unit matrix. We have used the facts that

$$\begin{aligned} (z_1 + z_2)^* &= [(x_1 + x_2) + i(y_1 + y_2)]^* \\ &= (x_1 + x_2) - i(y_1 + y_2) \\ &= z_1^* + z_2^* \end{aligned}$$

and

$$\begin{aligned} (z_1 z_2)^* &= [(x_1 + iy_1)(x_2 + iy_2)]^* \\ &= [x_1 x_2 - y_1 y_2 + i(x_1 y_2 + x_2 y_1)]^* \\ &= x_1 x_2 - y_1 y_2 - i(x_1 y_2 + x_2 y_1) \\ &= (x_1 - iy_1)((x_2 - iy_2)) \\ &= z_1^* z_2^*. \end{aligned}$$

- ii) For  $-1$  and  $T$ :

$$\begin{aligned} \mathbf{1} &= AA^{-1}, \\ \mathbf{1} &= (AA^{-1})^T, \\ \mathbf{1} &= (A^{-1})^T A^T, \\ (A^T)^{-1} &= (A^{-1})^T. \end{aligned}$$

Here we have used result

$$(AB)^T = B^T A^T$$

which can be proved as follows:

$$[(AB)^T]_{ik} = (AB)_{ki} = A_{kj} B_{ji} = B_{ij}^T A_{jk}^T = (B^T A^T)_{ik},$$

where we have used Einstein summation.

- iii) For  $-1$  and  $\dagger$ :

$$\begin{aligned} \mathbf{1} &= AA^{-1}, \\ \mathbf{1} &= (AA^{-1})^\dagger, \\ \mathbf{1} &= (A^{-1})^\dagger A^\dagger, \\ (A^\dagger)^{-1} &= (A^{-1})^\dagger. \end{aligned}$$

Here we have used result

$$(AB)^\dagger = B^\dagger A^\dagger$$

which can be proved as follows:

$$[(AB)^\dagger]_{ik} = [(AB)^*]_{ki} = [A^*B^*]_{ki} = A^*_{kj}B^*_{ji} = B^\dagger_{ij}A^\dagger_{jk} = (B^\dagger A^\dagger)_{ik} ,$$

where we have used Einstein summation. Note we haven't used the commuting property of transposing and complex conjugating in this proof, but we have supposed that Hermitian conjugation applies transposition first and then complex conjugation. Since we prove transposition and complex conjugation commute in part (iv) just below there is no concern.

iv) For  $*$  and  $T$

$$(A^*)^T = (A^T)^*$$

by inspection. But if you really need a tedious proof, then behold:

$$[(A^T)^*]_{ij} = [(A^T)_{ij}]^* = (A_{ji})^* = (A^*)_{ji} = [(A^*)^T]_{ij} .$$

Note

$$(A^*)^T = (A^T)^* = A^\dagger .$$

v) For  $*$  and  $\dagger$ :

$$(A^*)^\dagger = [(A^*)^T]^* = (A^\dagger)^* ,$$

where we have used the fact that transposing and complex conjugating commute, and thus that Hermitian conjugation does not care which order they are applied in.

vi) For  $T$  and  $\dagger$ :

$$(A^T)^\dagger = [(A^T)^*]^T = (A^\dagger)^T ,$$

where we have used the fact that transposing and complex conjugating commute, and thus that Hermitian conjugation does not care which order they are applied in.

**Redaction:** Jeffery, 2001jan01

007 qfull 00700 2 5 0 moderate thinking: square-integrable, inner product

**Extra keywords:** no analog Griffiths's problem, but discussion Gr-95-6, Gr2005-94-95

15. If  $f(x)$  and  $g(x)$  are square-integrable complex functions, then the inner product

$$\langle f|g \rangle = \int_{-\infty}^{\infty} f^* g dx$$

exists: i.e., is convergent to a finite value. In other words, that  $f(x)$  and  $g(x)$  are square-integrable is sufficient for the inner product's existence.

a) Prove the statement for the case where  $f(x)$  and  $g(x)$  are real functions. **HINT:** In doing this it helps to define a function

$$h(x) = \begin{cases} f(x) & \text{where } |f(x)| \geq |g(x)| \text{ (which we call the } f \text{ region);} \\ g(x) & \text{where } |f(x)| < |g(x)| \text{ (which we call the } g \text{ region),} \end{cases}$$

and show that it must be square-integrable. Then "squeeze"  $\langle f|g \rangle$ .

b) Now prove the statement for complex  $f(x)$  and  $g(x)$ . **HINTS:** Rewrite the functions in terms of their real and imaginary parts: i.e.,

$$f(x) = f_{\text{Re}}(x) + i f_{\text{Im}}(x)$$

and

$$g(x) = g_{\text{Re}}(x) + i g_{\text{Im}}(x) .$$

Now expand

$$\langle f|g \rangle = \int_{-\infty}^{\infty} f^* g dx$$



in the terms of the new real and imaginary parts and reduce the problem to the part (a) problem.

- c) Now for the easy part. Prove the converse of the statement is false. **HINT:** Find some trivial counterexample.
- d) Now another easy part. Say you have a vector space of functions  $\{f_i\}$  with inner product defined by

$$\int_{-\infty}^{\infty} f_j^* f_k dx .$$

Prove the following two statements are equivalent: 1) the inner product property holds; 2) the functions are square-integrable.

**SUGGESTED ANSWER:**

- a) Define

$$h(x) = \begin{cases} f(x) & \text{where } |f(x)| \geq |g(x)| \text{ (which we call the } f \text{ region);} \\ g(x) & \text{where } |f(x)| < |g(x)| \text{ (which we call the } g \text{ region).} \end{cases}$$

For the first case, we that

$$h^2 = f^2 = |f|^2 \geq |f||g|$$

and for the second that

$$h^2 = g^2 = |g|^2 \geq |f||g|$$

likewise. Thus in all cases

$$h^2 \geq |f||g| .$$

Clearly now,

$$\int_{-\infty}^{\infty} h^2 dx = \int_{f \text{ region}} f^2 dx + \int_{g \text{ region}} g^2 dx \leq \int_{-\infty}^{\infty} f^2 dx + \int_{-\infty}^{\infty} g^2 dx .$$

Thus,  $h(x)$  is square-integrable. Since for all  $x$

$$h(x)^2 \geq f(x)g(x) \geq -h(x)^2 ,$$

it follows that

$$\int_{-\infty}^{\infty} h^2 dx \geq \int_{-\infty}^{\infty} fg dx \geq - \int_{-\infty}^{\infty} h^2 dx .$$

Thus the inner product exists: QED.

- b) We first break the functions into real and imaginary parts

$$f(x) = f_{\text{Re}}(x) + i f_{\text{Im}}(x)$$

and

$$g(x) = g_{\text{Re}}(x) + i g_{\text{Im}}(x) .$$

Now

$$\int_{-\infty}^{\infty} f^* f dx = \int_{-\infty}^{\infty} f_{\text{Re}}^2 dx + \int_{-\infty}^{\infty} f_{\text{Im}}^2 dx$$

and

$$\int_{-\infty}^{\infty} g^* g dx = \int_{-\infty}^{\infty} g_{\text{Re}}^2 dx + \int_{-\infty}^{\infty} g_{\text{Im}}^2 dx ,$$

and so the part functions are also square-integrable. And now

$$\begin{aligned} \int_{-\infty}^{\infty} f^* g dx &= \int_{-\infty}^{\infty} f_{\text{Re}}^* g_{\text{Re}} dx + \int_{-\infty}^{\infty} f_{\text{Im}}^* g_{\text{Im}} dx - i \int_{-\infty}^{\infty} f_{\text{Im}}^* g_{\text{Re}} dx + i \int_{-\infty}^{\infty} f_{\text{Re}}^* g_{\text{Im}} dx \\ &= \int_{-\infty}^{\infty} f_{\text{Re}} g_{\text{Re}} dx + \int_{-\infty}^{\infty} f_{\text{Im}} g_{\text{Im}} dx - i \int_{-\infty}^{\infty} f_{\text{Im}} g_{\text{Re}} dx + i \int_{-\infty}^{\infty} f_{\text{Re}} g_{\text{Im}} dx . \end{aligned}$$

All the inner product integrals on the right-hand side of this equation just involve pure real functions that are all square-integrable, and so they all exist by the part (a) answer. Thus the inner product

$$\int_{-\infty}^{\infty} f^* g dx$$

exists: QED.

- c) Let  $f(x) = x^2$  and  $g(x) = 0$ . Clearly,

$$\int_{-\infty}^{\infty} f^* g dx = 0$$

exists, but

$$\int_{-\infty}^{\infty} f^* f dx = 2 \int_0^{\infty} x^2 dx$$

does not. This counterexample proves the converse is false.

I confess, I never saw the above case myself. It seems so trivial. I was thinking of cases where neither function is just zero. If neither is just zero, then one might guess that they could both be normalizable wave functions which must not be just zero everywhere. So a case where the inner product exists for non-zero functions, but one of the functions is not normalizable proves that the inner product existing for non-zero functions not guarantee normalizability.

For example, let  $f(x) = |x|$  and  $g(x) = (1/2)e^{-|x|}$ . Clearly,

$$\int_{-\infty}^{\infty} f^* g dx = \int_0^{\infty} x e^{-x} dx = -x e^{-x} \Big|_0^{\infty} + \int_0^{\infty} e^{-x} dx = 1 .$$

exists, but

$$\int_{-\infty}^{\infty} f^* f dx = 2 \int_0^{\infty} x^2 dx$$

does not. This counterexample proves the converse is false.

Another example is when  $f(x) = x^2$  and  $g(x) = e^{-x^2}$ . Clearly after using a table of integrals (Hod-313),

$$\int_{-\infty}^{\infty} f^* g dx = \frac{\sqrt{\pi}}{2}$$

exists, but

$$\int_{-\infty}^{\infty} f^* f dx = \int_{-\infty}^{\infty} x^4 dx$$

does not. This counterexample proves the converse is false too or even also.

Still another goody is when  $f(x) = 1/x$  and  $g(x) = x e^{-x^2}$ . Clearly after using a table of integrals (Hod-313),

$$\int_{-\infty}^{\infty} f^* g dx = \sqrt{\pi}$$

exists, but

$$\int_{-\infty}^{\infty} f^* f dx = \int_{-\infty}^{\infty} x^{-2} dx$$

does not.

- d) Say we have the vector space of functions  $\{f_i(x)\}$  for which statement 1 holds: i.e., the inner product property holds: i.e.,

$$\int_{-\infty}^{\infty} f_j^* f_k dx$$

exists for all functions in the vector space. The inner product also exists for  $j = k$ , and so the functions are square-integrable: statement 2 follows from statement 1. If statement 2 holds (i.e., the functions are all square-integrable), then it follows from the part (b) answer proof that the inner product property holds: viz., statement 1 follows from statement 2. Thus the two statements are equivalent.

You could put the statements in an if-and-only-if statement or necessary-and-sufficient statement. But I find those kind of statements hard to disentangle. I prefer saying the statements are equivalent: i.e., each one implies the other.

**Redaction:** Jeffery, 2001jan01

007 qfull 01000 2 3 0 moderate math: reduced SHO operator, Hermiticity

**Extra keywords:** (Gr-99:3.28), dimensionless simple harmonic oscillator Hamiltonian

16. Consider the operator

$$Q = -\frac{d^2}{dx^2} + x^2 .$$

- a) Show that  $f(x) = e^{-x^2/2}$  is an eigenfunction of  $Q$  and determine its eigenvalue.  
 b) Under what conditions, if any, is  $Q$  a Hermitian operator? **HINTS:** Recall

$$\langle g|Q^\dagger|f\rangle^* = \langle f|Q|g\rangle$$

is the defining relation for the Hermitian conjugate  $Q^\dagger$  of operator  $Q$ . You will have to write the matrix element  $\langle f|Q|g\rangle$  in the position representation and use integration by parts to find the conditions.

**SUGGESTED ANSWER:**

a) Behold:

$$Qf = \left(-\frac{d^2}{dx^2} + x^2\right)f = -\frac{d}{dx}(-xf) + x^2f = -x^2f + f + x^2f = f .$$

Thus  $f(x)$  is an eigenfunction and the eigenvalue is 1. By the by,  $Q$  is a dimensionless version of the simple harmonic oscillator Hamiltonian (see, e.g., Gr-37).

b) Behold:

$$\begin{aligned} \langle g|Q^\dagger|f\rangle^* &= \langle f|Q|g\rangle \\ &= \int_a^b f^* Qg \, dx \\ &= \int_a^b \left(-f^* \frac{d^2g}{dx^2} + f^* x^2 g\right) dx \\ &= \left(-f^* \frac{dg}{dx} + \frac{df^*}{dx} g\right) \Big|_a^b - \int_a^b g \frac{d^2f^*}{dx^2} dx + \int_a^b g x^2 f^* dx \\ &= \left(-f^* \frac{dg}{dx} + \frac{df^*}{dx} g\right) \Big|_a^b + \left(\int_a^b g^* Qf \, dx\right)^* \\ &= \left(-f^* \frac{dg}{dx} + \frac{df^*}{dx} g\right) \Big|_a^b + \langle g|Q|f\rangle^* , \end{aligned}$$

where we require  $f$  and  $g$  to be general square-integrable functions over the range  $[a, b]$ , we have used the general definition of the Hermitian conjugate, and we have used integration by parts twice. Clearly  $Q$  is Hermitian if the boundary condition term vanishes since then  $Q^\dagger = Q$ . For instance, if the boundaries were at minus and plus infinity, then the boundary condition term would have to vanish since the functions are square-integrable and so must be zero at minus and plus infinity. Or if periodic conditions were imposed on the functions, the boundary condition term would have to vanish again.

**Redaction:** Jeffery, 2001jan01

007 qfull 01100 2 5 0 moderate thinking: Hilbert space problems

**Extra keywords:** (Gr-103:3.33)

17. Do the following.

- a) Show explicitly that any linear combination of two functions in the Hilbert space  $L_2(a, b)$  is also in  $L_2(a, b)$ . (By explicitly, I mean don't just refer to the definition of a vector space which, of course requires the sum of any two vectors to be a vector.)
- b) For what values of real number  $s$  is  $f(x) = |x|^s$  in  $L_2(-a, a)$
- c) Show that  $f(x) = e^{-|x|}$  is in  $L_2 = L_2(-\infty, \infty)$ . Find the wavenumber space representation of  $f(x)$ : recall the wavenumber "orthonormal" basis states in the position representation are

$$\langle x|k\rangle = \frac{e^{ikx}}{\sqrt{2\pi}} .$$

**SUGGESTED ANSWER:**

- a) Given  $f$  and  $g$  in  $L_2(a, b)$ ,

$$\begin{aligned} \langle f+g|f+g\rangle &= \int_a^b (f+g)^*(f+g) dx \\ &= \int_a^b |f|^2 dx + \int_a^b |g|^2 dx + \int_a^b f^*g dx + \int_a^b g^*f dx \\ &= \langle f|f\rangle + \langle g|g\rangle + \langle f|g\rangle + \langle g|f\rangle . \end{aligned}$$

The inner products  $\langle f|f\rangle$  and  $\langle g|g\rangle$  exist by hypothesis. And their existence by theorem (see Gr-95-96) verifies that  $\langle f|g\rangle$  and  $\langle g|f\rangle$  exist. Thus  $\langle f+g|f+g\rangle$  exists and  $f+g$  are in the Hilbert space.

- b) Behold:

$$\langle f|f\rangle = 2 \int_0^a x^{2s} dx = 2 \times \begin{cases} \frac{x^{2s+1}}{2s+1} \Big|_0^a & \text{for } s \neq -1/2; \\ \ln(x) \Big|_0^a & \text{for } s = -1/2. \end{cases}$$

Clearly the integral only exists for  $s > -1/2$ . It's value when it exists is  $2a^{2s+1}/(2s+1)$ .

- c) Behold:

$$\langle f|f\rangle = 2 \int_0^\infty e^{-2x} dx = 1 .$$

Thus  $\langle f|f\rangle$  exists and  $f$  is in  $L_2$ .

Behold:

$$\begin{aligned} |f\rangle &= \int_{-\infty}^\infty dx |x\rangle \langle x|f\rangle , \\ \langle k|f\rangle &= \int_{-\infty}^\infty dx \langle k|x\rangle \langle x|f\rangle , \\ f(k) &= \int_{-\infty}^\infty dx \frac{e^{-ikx}}{\sqrt{2\pi}} f(x) = \int_{-\infty}^\infty dx \frac{e^{-ikx}}{\sqrt{2\pi}} e^{-|x|} \\ &= \sqrt{\frac{1}{2\pi}} \left[ \int_0^\infty dx e^{-(ik+1)x} + \int_0^\infty dx e^{-(ik+1)x} \right] \\ &= \sqrt{\frac{1}{2\pi}} \left[ \frac{e^{-(ik+1)x}}{-(-ik+1)} \Big|_0^\infty + \frac{e^{-(ik+1)x}}{-(ik+1)} \Big|_0^\infty \right] \\ &= \sqrt{\frac{2}{\pi}} \frac{1}{1+k^2} . \end{aligned}$$

18. Some general operator and vector identities should be proven. Recall the definition of the Hermitian conjugate of general operator  $Q$  is given by

$$\langle \alpha | Q | \beta \rangle = \langle \beta | Q^\dagger | \alpha \rangle^* ,$$

where  $|\alpha\rangle$  and  $|\beta\rangle$  are general vectors.

- a) Prove that the bra corresponding to ket vector  $Q|\beta\rangle$  is  $\langle \beta | Q^\dagger$  for general  $Q$  and  $|\beta\rangle$ . **HINT:** Consider general vector  $|\alpha\rangle$  and the inner product

$$\langle \alpha | Q | \beta \rangle$$

and work your way by valid steps to

$$\langle \beta | Q^\dagger | \alpha \rangle^*$$

and that completes the proof since

$$\langle \alpha | \gamma \rangle = \langle \gamma | \alpha \rangle^*$$

for general vectors  $|\alpha\rangle$  and  $|\gamma\rangle$ .

- b) Show that the Hermitian conjugate of a scalar  $c$  is just its complex conjugate.  
c) Prove for operators, not matrices, that

$$(AB)^\dagger = B^\dagger A^\dagger .$$

The result is, of course, consistent with matrix representations of these operators. But there are representations in which the operators are not matrices: e.g., the momentum operator in the position representation is differentiating operator

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x} .$$

Our proof holds for such operators too since we've done the proof in the general operator-vector formalism.

- d) Generalize the proof in part (c) for an operator product of any number.  
e) Prove that  $(A + B)^\dagger = A^\dagger + B^\dagger$ .  
f) Prove that  $c[A, B]$  is a Hermitian operator for Hermitian  $A$  and  $B$  only when  $c$  is pure imaginary constant.

### SUGGESTED ANSWER:

- a) Behold:

$$\langle \alpha | Q | \beta \rangle = \langle \beta | Q^\dagger | \alpha \rangle^*$$

by the definition of the Hermitian conjugate. And that completes the proof.

- b) Let  $|\alpha\rangle$ ,  $|\beta\rangle$  and  $c$  be general. Just using the vector rules that we have

$$\langle \alpha | c^\dagger | \beta \rangle = \langle \beta | c | \alpha \rangle^* = c^* \langle \beta | \alpha \rangle^* = c^* \langle \alpha | \beta \rangle = \langle \alpha | c^* | \beta \rangle .$$

Thus  $c^\dagger = c^*$ .

- c) For general  $|\alpha\rangle$  and  $|\beta\rangle$ ,

$$\langle \beta | (AB)^\dagger | \alpha \rangle = \langle \alpha | AB | \beta \rangle^* = [(\langle \alpha | A)(B | \beta \rangle)]^* = \langle \beta | B^\dagger A^\dagger | \alpha \rangle$$

where we have used the definition of the Hermitian conjugate operator and the fact that the bra corresponding to  $Q|\gamma\rangle$  for any operator  $Q$  and ket  $|\gamma\rangle$  is  $\langle \gamma | Q^\dagger$ . Since  $|\alpha\rangle$  and  $|\beta\rangle$  are general, it follows that

$$(AB)^\dagger = B^\dagger A^\dagger .$$

d) Behold:

$$(ABCD\dots)^\dagger = (BCD\dots)^\dagger A^\dagger = (CD\dots)^\dagger B^\dagger A^\dagger = \dots D^\dagger C^\dagger B^\dagger A^\dagger .$$

e) Behold:

$$\langle \alpha | (A + B)^\dagger | \beta \rangle = \langle \beta | (A + B) | \alpha \rangle^* = \langle \beta | A | \alpha \rangle^* + \langle \beta | B | \alpha \rangle^* = \langle \alpha | A^\dagger | \beta \rangle + \langle \alpha | B^\dagger | \beta \rangle ,$$

and given that  $|\alpha\rangle$  and  $|\beta\rangle$  are general, it follows that

$$(A + B)^\dagger = A^\dagger + B^\dagger .$$

Thus, the Hermitian conjugate operation is distributive over addition.

f) Behold:

$$(c[A, B])^\dagger = (cAB)^\dagger - (cBA)^\dagger = B^\dagger A^\dagger c^\dagger - A^\dagger B^\dagger c^\dagger = BAc^* - ABc^* = -c^*[A, B] .$$

If  $c^* = -c$ , then  $c$  is pure imaginary and

$$(c[A, B])^\dagger = c[A, B] .$$

Thus  $(c[A, B])$  is Hermitian only for  $c$  pure imaginary.

**Redaction:** Jeffery, 2001jan01

007 qfull 01400 2 5 0 moderate thinking: bra ket projector completeness

**Extra keywords:** (Gr-118:3.57) See also CT-115, 138

19. For an inner product vector space there is some rule for calculating the inner product of two general vectors: an inner product being a complex scalar. If  $|\alpha\rangle$  and  $|\beta\rangle$  are general vectors, then their inner product is denoted by

$$\langle \alpha | \beta \rangle ,$$

where in general the order is significant. Obviously different rules can be imagined for a vector space which would lead to different values for the inner products. But the rule must have three basic properties:

- (1)  $\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle^* ,$   
 (2)  $\langle \alpha | \alpha \rangle \geq 0 ,$  where  $\langle \alpha | \alpha \rangle = 0$  if and only if  $|\alpha\rangle = |0\rangle ,$

and

- (3)  $\langle \alpha | (b|\beta\rangle + c|\gamma\rangle) \rangle = b\langle \alpha | \beta \rangle + c\langle \alpha | \gamma \rangle ,$

where  $|\alpha\rangle$ ,  $|\beta\rangle$ , and  $|\gamma\rangle$  are general vectors of the vector space and  $b$  and  $c$  are general complex scalars.

There are some immediate corollaries of the properties. First, if  $\langle \alpha | \beta \rangle$  is pure real, then

$$\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle .$$

Second, if  $\langle \alpha | \beta \rangle$  is pure imaginary, then

$$\langle \beta | \alpha \rangle = -\langle \alpha | \beta \rangle .$$

Third, if

$$|\delta\rangle = b|\beta\rangle + c|\gamma\rangle ,$$

then

$$\langle \delta | \alpha \rangle^* = \langle \alpha | \delta \rangle = b\langle \alpha | \beta \rangle + c\langle \alpha | \gamma \rangle$$

which implies

$$\langle \delta | \alpha \rangle = b^*\langle \beta | \alpha \rangle + c^*\langle \gamma | \alpha \rangle .$$

This last result makes

$$\left( \langle \beta | b^* + \langle \gamma | c^* \right) | \alpha \rangle = b^*\langle \beta | \alpha \rangle + c^*\langle \gamma | \alpha \rangle$$

a meaningful expression. The 3rd rule for a vector product inner space and last corollary together mean that the distribution of inner product multiplication over addition happens in the normal way one is used to.

Dirac had the happy idea of defining dual space vectors with the notation  $\langle\alpha|$  for the dual vector of  $|\alpha\rangle$ :  $\langle\alpha|$  being called the bra vector or bra corresponding to  $|\alpha\rangle$ , the ket vector or ket: “bra” and “ket” coming from “bracket.” Mathematically, the bra  $\langle\alpha|$  is a linear function of the vectors. It has the property of acting on a general vector  $|\beta\rangle$  and yielding a complex scalar: the scalar being exactly the inner product  $\langle\alpha|\beta\rangle$ .

One immediate consequence of the bra definition can be drawn. Let  $|\alpha\rangle$ ,  $|\beta\rangle$ , and  $a$  be general and let

$$|\alpha'\rangle = a|\alpha\rangle .$$

Then

$$\langle\alpha'|\beta\rangle = \langle\beta|\alpha'\rangle^* = a^*\langle\beta|\alpha\rangle^* = a^*\langle\alpha|\beta\rangle$$

implies that the bra corresponding to  $|\alpha'\rangle$  is given by

$$\langle\alpha'| = a^*\langle\alpha| = \langle\alpha|a^* .$$

The use of bra vectors is perhaps unnecessary, but they do allow some operations and properties of inner product vector spaces to be written compactly and intelligibly. Let's consider a few nice uses.

- a) The projection operator or projector on to unit vector  $|e\rangle$  is defined by

$$P_{\text{op}} = |e\rangle\langle e| .$$

This operator has the property of changing a vector into a new vector that is  $|e\rangle$  times a scalar. It is perfectly reasonable to call this new vector the component of the original vector in the direction of  $|e\rangle$ : this definition of component agrees with our 3-dimensional Euclidean definition of a vector component, and so is a sensible generalization of that the 3-dimensional Euclidean definition. This generalized component would also be the contribution of a basis of which  $|e\rangle$  is a member to the expansion of the original vector: again the usage of the word component is entirely reasonable. In symbols

$$P_{\text{op}}|\alpha\rangle = |e\rangle\langle e|\alpha\rangle = a|e\rangle ,$$

where  $a = \langle e|\alpha\rangle$ .

Show that  $P_{\text{op}}^2 = P_{\text{op}}$ , and then that  $P_{\text{op}}^n = P_{\text{op}}$ , where  $n$  is any integer greater than or equal to 1. **HINTS:** Write out the operators explicitly and remember  $|e\rangle$  is a unit vector.

- b) Say we have

$$P_{\text{op}}|\alpha\rangle = a|\alpha\rangle ,$$

where  $P_{\text{op}} = |e\rangle\langle e|$  is the projection operator on unit vector  $|e\rangle$  and  $|\alpha\rangle$  is unknown non-null vector. Solve for the **TWO** solutions for  $a$ . Then solve for the  $|\alpha\rangle$  vectors corresponding to these solutions. **HINTS:** Act on both sides of the equation with  $\langle e|$  to find an equation for one  $a$  value. This equation won't yield the 2nd  $a$  value—and that's the hint for finding the 2nd  $a$  value. Substitute the  $a$  values back into the original equation to determine the corresponding  $|\alpha\rangle$  vectors. Note one  $a$  value has a vast degeneracy in general: i.e., many vectors satisfy the original equation with that  $a$  value.

- c) The Hermitian conjugate of an operator  $Q$  is written  $Q^\dagger$ . The definition of  $Q^\dagger$  is given by the expression

$$\langle\beta|Q^\dagger|\alpha\rangle = \langle\alpha|Q|\beta\rangle^* ,$$

where  $|\alpha\rangle$  and  $|\beta\rangle$  are general vectors. Prove that the bra corresponding to ket  $Q|\beta\rangle$  must  $\langle\beta|Q^\dagger$  for general  $|\alpha\rangle$ . **HINTS:** Let  $|\beta'\rangle = Q|\beta\rangle$  and substitute this for  $Q|\beta\rangle$  in the defining equation of the Hermitian conjugate operator. Note operators are not matrices (although they can be represented as matrices in particular bases), and so you are not free to use purely matrix concepts: in particular the concepts of transpose and complex conjugation of operators are not generally meaningful.

d) Say we define a particular operator  $Q$  by

$$Q = |\phi\rangle\langle\psi| ,$$

where  $|\phi\rangle$  and  $|\psi\rangle$  are general vectors. Solve for  $Q^\dagger$ . Under what condition is

$$Q^\dagger = Q ?$$

When an operator equals its Hermitian conjugate, the operator is called Hermitian just as in the case of matrices.

e) Say  $\{|e_i\rangle\}$  is an orthonormal basis. Show that

$$|e_i\rangle\langle e_i| = \mathbf{1} ,$$

where we have used Einstein summation and  $\mathbf{1}$  is the unit operator. **HINT:** Expand a general vector  $|\alpha\rangle$  in the basis.

### SUGGESTED ANSWER:

a) Behold:

$$P_{\text{op}}^2 = |e\rangle\langle e|e\rangle\langle e| = |e\rangle\langle e| = P_{\text{op}} ,$$

where we have used the normalization of  $|e\rangle$ . Now

$$P_{\text{op}}^n = |e\rangle\langle e|e\rangle^{n-1}\langle e| = |e\rangle\langle e| = P_{\text{op}} ,$$

where we have used the normalization of  $|e\rangle$ . I would actually accept that  $P_{\text{op}}^n = P_{\text{op}}$  is true by inspection given that  $P_{\text{op}}^2 = P_{\text{op}}$  is true.

b) Well

$$\langle e|P_{\text{op}}|\alpha\rangle = a\langle e|\alpha\rangle$$

leads to

$$\langle e|\alpha\rangle = a\langle e|\alpha\rangle .$$

If  $\langle e|\alpha\rangle \neq 0$ ,  $a = 1$ . If  $\langle e|\alpha\rangle = 0$ ,  $a = 0$  in order for

$$P_{\text{op}}|\alpha\rangle = |e\rangle\langle e|\alpha\rangle = 0 = a|\alpha\rangle$$

to hold remembering that  $|\alpha\rangle$  is not null. If  $a = 1$ , then

$$|e\rangle\langle e|\alpha\rangle = |\alpha\rangle$$

or

$$|\alpha\rangle = |e\rangle\langle e|\alpha\rangle .$$

Thus  $|\alpha\rangle$  points in the  $|e\rangle$  direction. If  $a = 0$ , then

$$\langle e|\alpha\rangle = 0 .$$

Any vector  $|\alpha\rangle$  perpendicular to  $|e\rangle$  is a solution.

We have, in fact, solved the eigenvalue problem for the  $P_{\text{op}}$  operator. The eigenvalues are 1 and 0 and the corresponding normalized eigenvectors are  $|e\rangle$  and

$$\frac{|\beta\rangle - |e\rangle\langle e|\beta\rangle}{\|(|\beta\rangle - |e\rangle\langle e|\beta\rangle)\|} ,$$

where  $|\beta\rangle$  is general non-null vector. This set of eigenvectors is actually complete. General vector  $|\beta\rangle$  can be expanded so

$$|\beta\rangle = |e\rangle\langle e|\beta\rangle + (|\beta\rangle - |e\rangle\langle e|\beta\rangle) .$$



Act on this vector with  $|e\rangle$  and one gets  $\langle e|\beta\rangle$ . Act on it with any  $|e_\perp\rangle$  orthogonal to  $|e\rangle$  and one gets  $\langle e_\perp|\beta\rangle$

c) Well

$$\langle\beta|Q^\dagger|\alpha\rangle = \langle\alpha|\beta'\rangle^* = \langle\beta'|a\rangle.$$

Since  $a$  is general we must interpret

$$\langle\beta'| = \langle\beta|Q^\dagger.$$

d) Well

$$\langle\beta|Q^\dagger|\alpha\rangle = \langle\alpha|Q|\beta\rangle^* = \langle\alpha|\phi\rangle^*\langle\psi|\beta\rangle^* = \langle\beta|\psi\rangle\langle\phi|\alpha\rangle,$$

and so

$$Q^\dagger = |\psi\rangle\langle\phi|.$$

If  $|\psi\rangle = |\phi\rangle$ , then  $Q^\dagger = |\phi\rangle\langle\phi| = Q$ , and  $Q$  would be a Hermitian operator.

e) Since the basis is a basis

$$|\alpha\rangle = a_i|e_i\rangle,$$

where the coefficients are given by

$$a_i = \langle e_i|\alpha\rangle.$$

Thus

$$|\alpha\rangle = |e_i\rangle\langle e_i|\alpha\rangle,$$

and so we must identify

$$|e_i\rangle\langle e_i| = \mathbf{1}.$$

This may seem trivial, but it is a great notational convenience. One can insert the unit operator  $\mathbf{1}$  in anywhere one likes in expressions, and so one can insert  $|e_i\rangle\langle e_i|$  in those places too. This makes expanding in various bases notationally very simple and obvious. The operator  $|e_i\rangle\langle e_i|$  can be considered the projection operator onto a basis.

**Redaction:** Jeffery, 2001jan01

008 qmult 00090 1 4 5 easy deducto-memory: example Hilbert space

20. "Let's play *Jeopardy!* For \$100, the answer is: A space of all square-integrable functions on the  $x$  interval  $(a, b)$ ."

What is a \_\_\_\_\_, Alex?

- a) non-inner product vector space    b) non-vector space    c) Dilbert space  
d) Dogbert space    e) Hilbert space

**SUGGESTED ANSWER:** (e)

**Wrong answers:**

- c) Now if this is late in the day: Dilbert was this ...

**Redaction:** Jeffery, 2001jan01

008 qmult 00100 1 1 3 easy memory: complex conjugate of scalar product

21. The scalar product  $\langle f|g\rangle^*$  in general equals:

- a)  $\langle f|g\rangle$ .    b)  $i\langle f|g\rangle$ .    c)  $\langle g|f\rangle$ .    d)  $\langle f|i|g\rangle$ .    e)  $\langle f|(-i)|g\rangle$ .

**SUGGESTED ANSWER:** (c)

**Wrong Answers:**

- a) This is true only if  $\langle f|g\rangle^*$  is pure real.

**Redaction:** Jeffery, 2001jan01

008 qmult 00200 1 4 3 easy deducto-memory: what operators do

22. "Let's play *Jeopardy!* For \$100, the answer is: It changes a vector into another vector."

What is a/an \_\_\_\_\_, Alex?

- a) wave function    b) scalar product    c) operator    d) bra    e) telephone operator

**SUGGESTED ANSWER:** (c)

**Wrong answers:**

- e) The adjective renders this incorrect.

**Redaction:** Jeffery, 2001jan01

008 qmult 00300 2 1 5 moderate memory: Hermitian conjugate of product

23. Given general operators  $A$  and  $B$ ,  $(AB)^\dagger$  equals:

- a)  $AB$ .   b)  $A^\dagger B^\dagger$ .    c)  $A$ .    d)  $B$ .    e)  $B^\dagger A^\dagger$ .

**SUGGESTED ANSWER:** (e) Using the operator definition of the Hermitian conjugate, the proof is

$$\langle \Psi | (AB)^\dagger | \chi \rangle = \langle \chi | AB | \Psi \rangle^* = \langle \Psi | B^\dagger A^\dagger | \chi \rangle .$$

Recall the bra corresponding to  $Q|\gamma\rangle$  is  $\langle \gamma|Q^\dagger$  in general.

**Wrong Answers:**

- a) Only if  $AB$  is Hermitian.  
 b) Only if  $A^\dagger$  and  $B^\dagger$  commute.  
 c) Only in some special case: most easily if  $A$  Hermitian and  $B^\dagger = 1$ .  
 d) Only in some special case: most easily if  $B$  Hermitian and  $A^\dagger = 1$ .

**Redaction:** Jeffery, 2001jan01

008 qmult 00400 2 5 5 moderate thinking: general Hermitian conjugation

24. The Hermitian conjugate of the operator  $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A$  (with  $\lambda$  a scalar and  $A$  an operator) is:

- a)  $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A$ .    b)  $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A^\dagger$ .    c)  $A|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda^*$ .    d)  $A|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda$ .  
 e)  $A^\dagger|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda^*$ .

**SUGGESTED ANSWER:** (e) Recall

$$(AB)^\dagger = B^\dagger A^\dagger .$$

This generalizes immediately to

$$(ABC\dots)^\dagger = (BC\dots)^\dagger A^\dagger = (C\dots)^\dagger A^\dagger B^\dagger = \dots C^\dagger B^\dagger A^\dagger .$$

Now the Hermitian conjugate of scalars  $\lambda$  and  $\langle\chi|\psi\rangle$  are  $\lambda^*$  and  $\langle\psi|\chi\rangle$ , respectively. For proof consider scalar  $c$  and general vectors  $|\alpha\rangle$  and  $|\beta\rangle$ :

$$\langle\alpha|c^\dagger|\beta\rangle = \langle\beta|c|\alpha\rangle^* = c^*\langle\beta|\alpha\rangle^* = c^*\langle\alpha|\beta\rangle = \langle\alpha|c^*|\beta\rangle ,$$

and so  $c^\dagger = c^*$ . The Hermitian conjugate of operator  $|\phi\rangle\langle\ell|$  is  $|\ell\rangle\langle\psi|$ . For a proof consider the general vectors  $|\alpha\rangle$  and  $|\beta\rangle$ :

$$\langle\alpha|\phi\rangle\langle\ell|\beta\rangle = \langle\phi|\alpha\rangle^*\langle\beta|\ell\rangle^* = \langle\beta|\ell\rangle^*\langle\phi|\alpha\rangle^* = (\langle\beta|\ell\rangle\langle\phi|\alpha\rangle)^* ,$$

and that completes the proof. Now put all the above results together and answer (e) follows. Remember scalars can be commuted freely.

**Wrong Answers:**

- a) This is just the same thing all over again.

**Redaction:** Jeffery, 2001jan01

008 qmult 00500 1 1 5 easy memory: compatible observables

25. Compatible observables:

- a) anticommute.    b) are warm and cuddly with each other.    c) have no hair.    d) have no complete simultaneous orthonormal basis.    e) commute.

**SUGGESTED ANSWER:** (e)

**Wrong Answers:**

- d) Actually they are guaranteed to have a complete simultaneous basis which can (if it isn't already) be orthonormalized.

**Redaction:** Jeffery, 2001jan01

008 qmult 00600 1 1 3 easy memory: parity operator

26. The parity operator  $\Pi$  acting on  $f(x)$  gives:

- $df/dx$ .    b)  $1/f(x)$ .    c)  $f(-x)$ .    d) 0.    e) a spherical harmonic.

**SUGGESTED ANSWER:** (c)

**Wrong Answers:**

- e) Whoa, fella.

**Redaction:** Jeffery, 2001jan01

008 qmult 00700 1 4 3 easy deducto-memory: braket expectation value

27. Given the position representation for an expectation value

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi(x)^* Q \Psi(x) dx ,$$

what is the braket representation?

- a)  $\langle Q | \Psi^* | Q \rangle$ .    b)  $\langle \Psi^* | Q | \Psi \rangle$ .    c)  $\langle \Psi | Q | \Psi \rangle$ .    d)  $\langle \Psi | Q^\dagger | \Psi \rangle$ .    e)  $\langle Q | \Psi | Q \rangle$ .

**SUGGESTED ANSWER:** (c)

**Wrong Answers:**

- d) Only true if  $Q$  is Hermitian.

**Redaction:** Jeffery, 2001jan01

008 qmult 00800 1 4 3 easy deducto-memory: Hermitian eigenproblem

28. What are the three main properties of the solutions to a Hermitian operator eigenproblem?

- a) (i) The eigenvalues are pure **IMAGINARY**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors **DO NOT** span all space.
- b) (i) The eigenvalues are pure **REAL**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors span all space in **ALL** cases.
- c) (i) The eigenvalues are pure **REAL**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors span all space for **ALL FINITE-DIMENSIONAL** spaces. In infinite dimensional cases they may or may not span all space. It is quantum mechanics postulate that the eigenvectors of an observable (which is a Hermitian operator) span all space.
- d) (i) The eigenvalues are pure **IMAGINARY**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors span all space in **ALL FINITE-DIMENSIONAL** spaces. In infinite dimensional cases they may or may not span all space.
- e) (i) The eigenvalues are pure **REAL**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized.

**SUGGESTED ANSWER:** (c)

**Wrong Answers:**

- b) I once thought this was true, but Griffiths (Gr-93, Gr-99) set me straight.  
e) Just checking to see if you can count.

**Redaction:** Jeffery, 2001jan01

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008 qmult 00900 1 4 5 easy deducto-memory: definition observable

29. “Let’s play *Jeopardy!* For \$100, the answer is: A physically significant Hermitian operator possessing a complete set of eigenvectors.”

What is a/an \_\_\_\_\_, Alex?

- a) conjugate    b) bra    c) ket    d) inobservable    e) observable

**SUGGESTED ANSWER:** (e)

**Wrong answers:**

- d) Exactly wrong.

**Redaction:** Jeffery, 2001jan01

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008 qmult 01000 1 4 4 easy deducto-memory: time-energy inequality

30. In the precisely-formulated time-energy inequality, the  $\Delta t$  is:

- a) the standard deviation of time.  
 b) the standard deviation of energy.  
 c) a Hermitian operator.  
 d) the characteristic time for an observable’s value to change by one standard deviation.  
 e) the characteristic time for the system to do nothing.

**SUGGESTED ANSWER:** (d) Characteristic time is often defined precisely as the time for a change if the rate of change is assumed to be constant. This is the usage in the precisely-formulated time-energy inequality. Note that the longest-answer-is-right rule is obeyed here.

**Wrong Answers:** itemitema) Nah. That’s what it looks like since by convention it’s written with the same symbol used for often standard deviation.

- b) Nah.  
 c) It’s just a number.  
 e) Seems a bit vague.

**Redaction:** Jeffery, 2001jan01

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008 qmult 02000 1 1 5 easy memory: common eigensets

**Extra keywords:** See CT-140ff

31. The statements “two observables commute” and “a common eigenset can be constructed for two observables” are

- a) in flat contradiction.    b) unrelated.    c) in non-intersecting Venn diagrams.  
 d) irrelevant in relation to each other.    e) are equivalent in the sense that one implies the other.

**SUGGESTED ANSWER:** (e) Another triumph for the longest answer is right rule.

**Wrong Answers:**

- a) Exactly wrong.  
 c) I’m not sure what this means.

**Redaction:** Jeffery, 2001jan01

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008 qfull 00030 2 5 0 moderate thinking: Hermiticity and expectation values

**Extra keywords:** (Gr-94:3.21)

32. Recall the definition of Hermitian conjugate for a general operator  $Q$  is

$$\langle \alpha | Q | \beta \rangle = \langle \beta | Q^\dagger | \alpha \rangle^* ,$$

where  $|\alpha\rangle$  and  $|\beta\rangle$  are general vectors. If  $Q$  is Hermitian,

$$Q^\dagger = Q :$$

i.e.,  $Q$  is its own Hermitian conjugate.

- a) If  $Q$  is Hermitian, prove that the expectation value of a general vector  $|\gamma\rangle$ ,

$$\langle\gamma|Q|\gamma\rangle,$$

is pure real.

- b) If the expectation value

$$\langle\gamma|Q|\gamma\rangle$$

is always pure real for general  $|\gamma\rangle$ , prove that  $Q$  is Hermitian. The statement to be proven is the converse of the statement in part (a). **HINT:** First show that

$$\langle\gamma|Q|\gamma\rangle = \langle\gamma|Q^\dagger|\gamma\rangle.$$

Then let  $|\alpha\rangle$  and  $|\beta\rangle$  be general vectors and construct a vector  $|\xi\rangle = |\alpha\rangle + c|\beta\rangle$ , where  $c$  is a general complex scalar. Note that the bra corresponding to  $c|\beta\rangle$  is  $c^*\langle\beta|$ . Expand both sides of

$$\langle\xi|Q|\xi\rangle = \langle\xi|Q^\dagger|\xi\rangle,$$

and then keep simplifying both sides making use of the first thing proven and the definition of a Hermitian conjugate. It may be useful to note that

$$(A^\dagger)^\dagger = A \quad \text{and} \quad (A + B)^\dagger = A^\dagger + B^\dagger,$$

where  $A$  and  $B$  are general operators and You should be able to construct an expression where choosing  $c = 1$  and then  $c = i$  requires  $Q = Q^\dagger$ .

- c) What simple statement follows from the proofs in parts (a) and (b)?

**SUGGESTED ANSWER:**

- a) Well

$$\langle\gamma|Q|\gamma\rangle = \langle\gamma|Q^\dagger|\gamma\rangle^*$$

by the general definition of Hermitian conjugation. But since  $Q^\dagger = Q$ , we have

$$\langle\gamma|Q|\gamma\rangle = \langle\gamma|Q|\gamma\rangle^*.$$

Since the expectation value is equal to its own complex conjugate, it is pure real: i.e.,  $\langle\gamma|Q|\gamma\rangle$  is pure real.

- b) First note for general  $|\gamma\rangle$  that

$$\langle\gamma|Q|\gamma\rangle = \langle\gamma|Q^\dagger|\gamma\rangle^* = \langle\gamma|Q^\dagger|\gamma\rangle,$$

where we have used the definition of the Hermitian conjugate and then the fact that by assumption  $\langle\gamma|Q|\gamma\rangle$  is pure real which implies that  $\langle\gamma|Q^\dagger|\gamma\rangle^*$  is pure real too.

For general vectors  $|\alpha\rangle$  and  $|\beta\rangle$ , we define

$$|\xi\rangle = |\alpha\rangle + c|\beta\rangle,$$

where  $c$  is a general complex number. The point of this definition is to exploit our statement above for the general vector  $|\gamma\rangle$  (which will hold for  $|\alpha\rangle$ ,  $|\beta\rangle$ , and  $|\xi\rangle$ ) and then the generality of  $|\alpha\rangle$  and  $|\beta\rangle$  to get a statement like

$$\langle\alpha|Q|\beta\rangle = \langle\alpha|Q^\dagger|\beta\rangle$$

which verifies  $Q^\dagger = Q$ —but we haven't got this statement yet. Why do we need the general complex constant  $c$ ? Well if you went through the steps without it, you would reach a point where you needed and then you'd go back and put it in.

Starting from

$$\langle\xi|Q|\xi\rangle = \langle\xi|Q^\dagger|\xi\rangle,$$

we proceed as follows

$$\begin{aligned}
\langle \xi|Q|\xi \rangle &= \langle \xi|Q^\dagger|\xi \rangle \\
\langle \alpha|Q|\alpha \rangle + |c|^2 \langle \beta|Q|\beta \rangle + c \langle \alpha|Q|\beta \rangle + c^* \langle \beta|Q|\alpha \rangle &= \langle \alpha|Q^\dagger|\alpha \rangle + |c|^2 \langle \beta|Q^\dagger|\beta \rangle + c \langle \alpha|Q^\dagger|\beta \rangle + c^* \langle \beta|Q^\dagger|\alpha \rangle \\
c \langle \alpha|Q|\beta \rangle + c^* \langle \beta|Q|\alpha \rangle &= c \langle \alpha|Q^\dagger|\beta \rangle + c^* \langle \beta|Q^\dagger|\alpha \rangle \\
0 &= c \langle \alpha|(Q - Q^\dagger)|\beta \rangle + c^* \langle \beta|(Q - Q^\dagger)|\alpha \rangle \\
0 &= c \langle \alpha|(Q - Q^\dagger)|\beta \rangle + c^* \langle \alpha|(Q - Q^\dagger)^\dagger|\beta \rangle^* \\
0 &= c \langle \alpha|(Q - Q^\dagger)|\beta \rangle - c^* \langle \alpha|(Q - Q^\dagger)|\beta \rangle^* . \tag{1}
\end{aligned}$$

Equation (1) must be true for all choices of  $c$ . If  $c = 1$ , then the real parts of equation (1) cancel identically, but imaginary parts give

$$\text{Im}[\langle \alpha|(Q - Q^\dagger)|\beta \rangle] = 0 .$$

If  $c = i$ , then the imaginary parts of equation (1) cancel identically since

$$i^2 - (-i)(-i) = i^2 - i^2 = 0$$

and we find that the real parts give

$$\text{Re}[\langle \alpha|(Q - Q^\dagger)|\beta \rangle] = 0 .$$

Thus, we obtain

$$\langle \alpha|(Q - Q^\dagger)|\beta \rangle = 0$$

or

$$\langle \alpha|Q|\beta \rangle = \langle \alpha|Q^\dagger|\beta \rangle .$$

Remember that  $|\alpha \rangle$  and  $|\beta \rangle$  are general, and thus

$$Q^\dagger = Q .$$

So  $Q$  must be Hermitian if all expectation values of  $Q$  are pure real.

We could actually do one more step to reconfirm the Hermiticity of  $Q$ . Using the definition of a Hermitian conjugate, we find

$$\langle \alpha|Q|\beta \rangle = \langle \alpha|Q^\dagger|\beta \rangle = \langle \beta|(Q^\dagger)^\dagger|\alpha \rangle^* = \langle \beta|Q|\alpha \rangle^*$$

or

$$\langle \alpha|Q|\beta \rangle = \langle \beta|Q|\alpha \rangle^*$$

which implies

$$Q^\dagger = Q .$$

I think that the above proof may be the simplest proof available.

Just to satisfy paranoia, we might prove some of the results we used in the above proof. First, that  $c^* \langle \beta$  is the bra corresponding to the ket  $c|\beta \rangle$  where  $c$  is a general complex number and  $c|\beta \rangle$  is a general vector. Consider general vector  $|\alpha \rangle$  and note that.

$$\langle \alpha|c|\beta \rangle = c \langle \alpha|\beta \rangle = c \langle \beta|\alpha \rangle^* = (c^* \langle \beta|\alpha \rangle)^* = \langle \beta|c^*|\alpha \rangle^*$$

Clearly,  $c^* \langle \beta$  is the bra corresponding to the ket  $c|\beta \rangle$ .

Second, that  $(Q^\dagger)^\dagger = Q$ . Consider general vectors  $|\alpha \rangle$  and  $|\beta \rangle$ . Now using the definition of the a Hermitian conjugate twice in a row

$$\langle \alpha|Q|\beta \rangle = \langle \beta|Q^\dagger|\alpha \rangle^* = \langle \alpha|(Q^\dagger)^\dagger|\beta \rangle ,$$

and so

$$(Q^\dagger)^\dagger = Q$$

QED.

Third, that  $(A + B)^\dagger = A^\dagger + B^\dagger$ . Consider general vectors  $|\alpha\rangle$  and  $|\beta\rangle$ . The proof is

$$\begin{aligned}\langle\alpha|(A + B)^\dagger|\beta\rangle^* &= \langle\beta|(A + B)|\alpha\rangle = \langle\beta|A|\alpha\rangle + \langle\beta|B|\alpha\rangle \\ &= \langle\alpha|A^\dagger|\beta\rangle^* + \langle\alpha|B^\dagger|\beta\rangle^* = (\langle\alpha|A^\dagger|\beta\rangle + \langle\alpha|B^\dagger|\beta\rangle)^* \\ &= \langle\alpha|(A^\dagger + B^\dagger)|\beta\rangle^* ,\end{aligned}$$

and thus

$$\langle\alpha|(A + B)^\dagger|\beta\rangle = \langle\alpha|(A^\dagger + B^\dagger)|\beta\rangle ,$$

and thus again

$$(A + B)^\dagger = A^\dagger + B^\dagger$$

QED.

- c) The above two proofs show that the statements of parts (a) and (b) are equivalent: each implies the other. We could phrase the situation with the sentence “if and only if  $Q$  is Hermitian is  $\langle\gamma|Q|\gamma\rangle$  pure real for general  $|\gamma\rangle$ .” Or we could say “it is necessary and sufficient that  $Q$  be Hermitian for  $\langle\gamma|Q|\gamma\rangle$  to be pure real for general  $|\gamma\rangle$ .” These ways of saying things always seem asymmetric and obscure to me. I prefer to say that the statements of parts (a) and (b) are equivalent.

**Redaction:** Jeffery, 2001jan01

008 qfull 00040 2 3 0 moderate math: solving an eigenproblem

**Extra keywords:** (Gr-94:3.22) also diagonalizing a matrix.

33. Consider

$$Q = \begin{pmatrix} 1 & 1 - i \\ 1 + i & 0 \end{pmatrix} .$$

In this problem, we will diagonalize this matrix: i.e., solve for its eigenvalues and eigenvectors. We also actually explicitly find the diagonal form—which is not usually necessary.

- a) Is  $Q$  Hermitian?
- b) Solve for the eigenvalues. Are they real?
- c) Determine the normalized eigenvectors  $\hat{a}$ . Since eigenvectors are not unique to within a phase factor, the marker insists that you arrange your eigenvectors so that the first component of each is 1. Are the eigenvectors orthogonal? **HINT:** The matrix equation for the eigenvectors is a homogeneous matrix equation with non-trivial solutions (i.e., solutions that are not just zeros) for the eigenvalues since the determinant of  $Q - \lambda I$  vanishes for those eigenvalues. However, 1 equation obtained from a  $N \times N$  homogeneous matrix problem is always not independent: there are only  $N - 1$  independent equations and one can only solve for  $N - 1$  components of the eigenvectors. So if you set the first component of the solution vector to be 1, the  $N - 1$  equations allow you to solve for the other components. This solution vector is a valid solution vector, but its overall scale is arbitrary. There is no determined scale for the eigenvectors of a homogeneous matrix problem: e.g.,  $k$  times solution vector  $\vec{a}$  is also a solution. But, in quantum mechanics, physical vectors should be normalized and the normalization constraint provides an  $N$ th independent equation, and thus allows a complete solution of the eigenvectors to within a global phase factor. Normalization doesn't set that global phase factor since it cancels out in the normalization equation. The global phase factor can be chosen arbitrarily for convenience. The global phase factor of a state no effect on the physics of the state.
- d) Obtaining the eigenvalues and eigenvectors is usually all that is meant by diagonalization, but one can actually transform the eigenvalue matrix equation into a matrix equation where the matrix is diagonal and the eigenvectors can be solved for by inspection. One component of an eigenvector is 1 and the other components are zero. How does one transform to diagonal form? Consider our matrix equation

$$Q\hat{a} = \lambda\hat{a} .$$

Multiply both sides by the transformation matrix  $U$  to obtain

$$UQ\hat{a} = \lambda U\hat{a}$$

which is obviously the same as

$$UQU^{-1}U\hat{a} = \lambda U\hat{a} .$$

If we define

$$\hat{a}' = U\hat{a} \quad \text{and} \quad Q' = UQU^{-1} ,$$

then the transformed matrix equation is just

$$Q'\hat{a}' = \lambda\hat{a}' .$$

Prove that the transformation matrix  $U$  that gives the diagonalized matrix  $Q'$  just consists of rows that are the Hermitian conjugates of the eigenvectors. Then find the diagonalized matrix itself and its eigenvalue.

- e) Compare the determinant  $\det|Q|$ , trace  $\text{Tr}(Q)$ , and eigenvalues of  $Q$  to those of  $Q'$ .  
 f) The matrix  $U$  that we considered in part (d) is actually unitary. This means that

$$U^\dagger = U^{-1} .$$

Satisfy yourself that this is true. Unitary transformations have the useful property that inner products are invariant under them. If the inner product has a physical meaning and in particular the magnitude of vector has a physical meaning, unitary transformations can be physically relevant. In quantum mechanics, the inner product of a normalized state vector with itself 1 and this should be maintained by all physical transformations, and so such transformations must be unitary. Prove that

$$\langle a'|b' \rangle = \langle a|b \rangle$$

where

$$|a'\rangle = U|a\rangle |b'\rangle = U|b\rangle$$

and  $U$  is unitary.

**SUGGESTED ANSWER:**

- a) Yes by inspection. But to be explicit

$$Q^\dagger = (Q^*)^T = \begin{pmatrix} 1 & 1+i \\ 1-i & 0 \end{pmatrix}^T \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix} = Q ,$$

where  $T$  is the transpose function. Thus,  $Q = Q^\dagger$ , and so  $Q$  is Hermitian.

- b) The eigen equation is

$$(1 - \lambda)(-\lambda) - 2 = \lambda^2 - \lambda - 2 = (\lambda - 2)(\lambda + 1) = 0 .$$

The eigenvalues are clearly

$$\lambda = -1 \quad \text{and} \quad \lambda = 2 .$$

The eigenvalues are both real as they should be for a Hermitian matrix.

- c) The equation for the eigenvector components is

$$a_1 + (1 - i)a_2 = \lambda a_1$$

from which we obtain the unnormalized expression

$$\vec{a}(\lambda) = \begin{pmatrix} 1 \\ \frac{\lambda - 1}{1 - i} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{(\lambda - 1)(1 + i)}{2} \end{pmatrix} .$$

The normalized eigenvectors are

$$\hat{a}(\lambda = 2) = \sqrt{\frac{2}{3}} \begin{pmatrix} 1 \\ \frac{1+i}{2} \end{pmatrix} \quad \text{and} \quad \hat{a}(\lambda = -1) = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -(1+i) \end{pmatrix} .$$



The eigenvectors are orthogonal by inspection.

Note normalized eigenvectors that are physically the same can look quite different because of global phase factors. For example,

$$\begin{aligned}\hat{a}(\lambda = 2) &= \sqrt{\frac{2}{3}} \begin{pmatrix} 1 \\ \frac{1+i}{2} \end{pmatrix} = (1+i) \sqrt{\frac{2}{3}} \begin{pmatrix} \frac{1-i}{2} \\ \frac{1}{2} \end{pmatrix} = \frac{(1+i)}{\sqrt{2}} \sqrt{\frac{1}{3}} \begin{pmatrix} 1-i \\ 1 \end{pmatrix} \\ &= e^{i\pi/4} \frac{1}{\sqrt{3}} \begin{pmatrix} 1-i \\ 1 \end{pmatrix} .\end{aligned}$$

The global phase factor  $e^{i\pi/4}$  can be dropped because it is physically irrelevant. Physical eigenvectors are unique only to within a global phase factor. Caveat markor.

d) Following the question lead-in, we define

$$U = \begin{pmatrix} \sqrt{\frac{2}{3}} & \frac{1-i}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & -\frac{1-i}{\sqrt{3}} \end{pmatrix} .$$

Because the eigenvectors are orthonormal, the inverse matrix  $U^{-1}$  constructed using the eigenvectors for columns. Thus, we obtain.

$$U^{-1} = \begin{pmatrix} \sqrt{\frac{2}{3}} & \frac{1}{\sqrt{3}} \\ \frac{1+i}{\sqrt{6}} & -\frac{1+i}{\sqrt{3}} \end{pmatrix} .$$

Obviously,

$$UU^{-1} = I ,$$

where  $I$  is the unit matrix. If we multiply both sides from the right by  $U$ , we get

$$UU^{-1}U = U ,$$

and so  $U^{-1}U = 1$  too as it should.

We now find the elements of  $Q'$ . Since

$$Q' = UQU^{-1} ,$$

we have

$$Q'_{ij} = U_{ik} Q_{k\ell} U_{\ell j}^{-1} = U_{ik} \lambda_j U_{k j}^{-1} = \lambda_j \delta_{ij} = \lambda_i \delta_{ij} ,$$

where we have used the eigenproblem property itself, the fact that  $UU^{-1} = \mathbf{1}$ , and Einstein summation (i.e., there is an implicit sum on repeated indexes. That

$$Q_{k\ell} U_{\ell j}^{-1} = \lambda_j U_{k j}^{-1}$$

takes a little cogitating on. But note that

$$Q_{k\ell} U_{\ell j}^{-1} = V_{kj}$$

where the columns of  $V$  are the columns of  $U^{-1}$  times the eigenvalue of the eigenvector that makes up that row.

The proof is complete since the  $U$  matrix constructed as required yields a diagonal matrix whose elements are the eigenvalues.

So  $Q'$  is the required diagonalized matrix. In our case,

$$Q' = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix} .$$

By inspection, the transformed eigenvectors are

$$\hat{a}(\lambda = 2) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \hat{a}(\lambda = -1) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

e) Well

$$\det|Q| = -2 = \det|Q'| , \quad \text{Tr}(Q) = 1 = \text{Tr}(Q') ,$$

and the eigenvalues of  $Q$  (i.e., 2 and  $-1$ ) are clearly the eigenvalues of  $Q'$ .

The above results are special cases of more general results. We can prove this.

Say  $S$  is a general transformation acting on general matrix  $A$ . Then

$$\begin{aligned} \det|SAS^{-1}| &= \det|S| \times \det|A| \times \det|S^{-1}| \\ &= \det|A| \times \det|S| \times \det|S^{-1}| \\ &= \det|A| \times \det|SS^{-1}| \\ &= \det|A| , \end{aligned}$$

where we have used well known determinant properties: see, e.g., Mih-657. We see that the determinant is generally invariant under a similarity transformation.

Now note that

$$\text{Tr}(ABC \dots Z) = A_{ij}B_{jk}C_{\ell m} \dots Z_{ni} = B_{jk}C_{\ell m} \dots Z_{ni}A_{ij} = \text{Tr}(BC \dots ZA) .$$

Thus trace is invariant under a cycling of the matrix product. Therefore

$$\text{Tr}(SAS^{-1}) = \text{Tr}(AS^{-1}S) = \text{Tr}(A) .$$

Thus trace is invariant under a similarity transformation.

The invariance of the eigenvalues holds for Hermitian matrices under unitary similarity transformations constructed from their eigenvectors. Consider Hermitian matrix  $H$  and unitary matrix  $U$  constructed from the eigenvectors of  $H$ . The  $i\ell$ th element of  $H' = UHU^{-1}$  is given by

$$H' = \sum_{jk} U_{ij}H_{jk}U_{k\ell}^{-1} = \sum_j U_{ij}\lambda_\ell U_{j\ell}^{-1} = \lambda_\ell \sum_j U_{ij}U_{j\ell}^{-1} = \lambda_\ell \delta_{i\ell} ,$$

where we have **NOT** used Einstein summation and where  $\lambda_\ell$  is the eigenvalue corresponding to the eigenvector in the  $\ell$ th column of  $U_{k\ell}^\dagger$ . Thus we find that  $H^d$  is diagonal with diagonal elements being the eigenvalues of  $H$ : these elements are the eigenvalues of  $H^d$  by inspection. Are eigenvalues invariant under general similarity transformations or general unitary similarity transformations. I'd guess not, but we've done enough proofs for now.

f) By inspection, the matrix  $U$  we found in part (d) is unitary.

Well for general vectors  $|a\rangle$  and  $|b\rangle$

$$\langle a|U|b\rangle = \langle b|U^\dagger|a\rangle^*$$

by the definition of the Hermitian conjugate. There in general the bra corresponding to ket  $U|b\rangle$  is  $\langle b|U^\dagger$ .

Now for general vectors  $|a\rangle$  and  $|b\rangle$ , we can write

$$\langle a'|b'\rangle = \langle a|U^\dagger U|b\rangle = \langle a|U^{-1}U|b\rangle = \langle a|b\rangle ,$$

where we have used the unitary nature of  $U$  (i.e.,  $U^\dagger = U^{-1}$ ).

**Redaction:** Jeffery, 2001jan01

34. Consider the observable  $Q$  and the general **NORMALIZED** vector  $|\Psi\rangle$ . By quantum mechanics postulate, the expectation of  $Q^n$ , where  $n \geq 0$  is some integer, for  $|\Psi\rangle$  is

$$\langle Q^n \rangle = \langle \Psi | Q^n | \Psi \rangle .$$

- a) Assume  $Q$  has a discrete spectrum of eigenvalues  $q_i$  and orthonormal eigenvectors  $|q_i\rangle$ . It follows from the general probabilistic interpretation postulate of quantum mechanics, that expectation value of  $Q^n$  for  $|\Psi\rangle$  is given by

$$\langle Q^n \rangle = \sum_i q_i^n |\langle q_i | \Psi \rangle|^2 .$$

Show that this expression for  $\langle Q^n \rangle$  also follows from the one in the preamble. What is  $\sum_i |\langle q_i | \Psi \rangle|^2$  equal to?

- b) Assume  $Q$  has a continuous spectrum of eigenvalues  $q$  and Dirac-orthonormal eigenvectors  $|q\rangle$ . (Dirac-orthonormal means that  $\langle q' | q \rangle = \delta(q' - q)$ , where  $\delta(q' - q)$  is the Dirac delta function. The term Dirac-orthonormal is all my own invention: it needed to be.) It follows from the general probabilistic interpretation postulate of quantum mechanics, that expectation value of  $Q^n$  for  $|\Psi\rangle$  is given by

$$\langle Q^n \rangle = \int dq q^n |\langle q | \Psi \rangle|^2 .$$

Show that this expression for  $\langle Q^n \rangle$  also follows from the one in the preamble. What is  $\int dq |\langle q | \Psi \rangle|^2$  equal to?

**SUGGESTED ANSWER:**

- a) Since the eigenvectors  $|q_i\rangle$  constitute a complete orthonormal set,

$$|\Psi\rangle = \sum_i |q_i\rangle \langle q_i | \Psi \rangle .$$

Thus

$$\begin{aligned} \langle Q^n \rangle &= \langle \Psi | Q^n | \Psi \rangle \\ &= \sum_i \langle \Psi | Q^n | q_i \rangle \langle q_i | \Psi \rangle \\ &= \sum_i \langle \Psi | q_i^n | q_i \rangle \langle q_i | \Psi \rangle \\ &= \sum_i q_i^n |\langle q_i | \Psi \rangle|^2 , \end{aligned}$$

and so everything is consistent. Since  $|\Psi\rangle$  is normalized, we find for  $n = 0$  that

$$\langle \Psi | \Psi \rangle = 1 = \sum_i |\langle q_i | \Psi \rangle|^2 .$$

- b) Since the eigenvectors  $|q\rangle$  constitute a complete Dirac-orthonormal set,

$$|\Psi\rangle = \int dq |q\rangle \langle q | \Psi \rangle .$$

Thus

$$\begin{aligned} \langle Q^n \rangle &= \langle \Psi | Q^n | \Psi \rangle \\ &= \int dq \langle \Psi | Q^n | q \rangle \langle q | \Psi \rangle \\ &= \int dq \langle \Psi | q^n | q \rangle \langle q | \Psi \rangle \\ &= \int dq q^n |\langle q | \Psi \rangle|^2 , \end{aligned}$$

and so everything is consistent. Since  $|\Psi\rangle$  is normalized, we find for  $n = 0$  that

$$\langle\Psi|\Psi\rangle = 1 = \int dq |\langle q|\Psi\rangle|^2.$$

**Redaction:** Jeffery, 2001jan01

008 qfull 00200 2 5 0 moderate thinking: simple commutator identities

35. Prove the following commutator identities.

- a)  $[A, B] = -[B, A]$ .
- b)  $\left[ \sum_i a_i A_i, \sum_j b_j B_j \right] = \sum_{ij} a_i b_j [A_i, B_j]$ , where the  $a_i$ 's and  $b_j$ 's are just complex numbers.
- c)  $[A, BC] = [A, B]C + B[A, C]$ .
- d)  $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$ . This has always seemed to me to be perfectly useless however true.
- e)  $(c[A, B])^\dagger = c^*[B^\dagger, A^\dagger]$ , where  $c$  is a complex number.
- f) The special case of the part (e) identity when  $A$  and  $B$  are Hermitian and  $c$  is pure imaginary. Is the operator in this special case Hermitian or anti-Hermitian?

**SUGGESTED ANSWER:**

a)  $[A, B] = AB - BA = -(BA - AB) = -[B, A]$ .

b) Behold:

$$\begin{aligned} \left[ \sum_i a_i A_i, \sum_j b_j B_j \right] &= \left( \sum_i a_i A_i \right) \left( \sum_j b_j B_j \right) - \left( \sum_j b_j B_j \right) \left( \sum_i a_i A_i \right) \\ &= \sum_{ij} a_i b_j A_i B_j - \sum_{ij} a_i b_j B_j A_i = \sum_{ij} a_i b_j (A_i B_j - B_j A_i) \\ &= \sum_{ij} a_i b_j [A_i, B_j]. \end{aligned}$$

c)  $[A, BC] = ABC - BCA = ABC - BAC + BAC - BCA = [A, B]C + B[A, C]$ .

d) Behold:

$$\begin{aligned} [A, [B, C]] + [B, [C, A]] + [C, [A, B]] &= (ABC - ACB - BCA + CBA) \\ &\quad + (BCA - BAC - CAB + ACB) \\ &\quad + (CAB - CBA - ABC + BAC) \\ &= 0. \end{aligned}$$

e) Behold:

$$(c[A, B])^\dagger = c^*(B^\dagger A^\dagger - A^\dagger B^\dagger) = c^*[B^\dagger, A^\dagger].$$

f) Using the parts (e) and (a) answers for  $A$  and  $B$  Hermitian and  $c$  pure imaginary,

$$(c[A, B])^\dagger = c^*[B^\dagger, A^\dagger] = -c[B, A] = c[A, B].$$

In this special case,  $c[A, B]$  is itself Hermitian. If  $c$  is pure real then  $c[A, B]$  is anti-Hermitian (see Gr-83).

**Redaction:** Jeffery, 2001jan01

008 qfull 00300 3 5 0 tough thinking: nontrivial commutator identities

**Extra keywords:** (Gr-111:3.41) but considerably extended.

36. Prove the following somewhat more difficult commutator identities.

a) Given

$$[B, [A, B]] = 0, \quad \text{prove} \quad [A, F(B)] = [A, B]F'(B),$$

where  $A$  and  $B$  are general operators aside from the given condition and  $F(B)$  is a general operator function of  $B$ . **HINTS:** Proof by induction is probably best. Recall that any function of an operator is (or is that should be) expandable in a power series of the operator: i.e.,

$$F(B) = \sum_{n=0}^{\infty} f_n B^n,$$

where  $f_n$  are constants.

b)  $[x, p] = i\hbar$ .

c)  $[x, p^n] = i\hbar np^{n-1}$ . **HINT:** Recall the part (a) answer.

d)  $[p, x^n] = -i\hbar nx^{n-1}$ . **HINT:** Recall the part (a) answer.

**SUGGESTED ANSWER:**

a) Any operator function can be expanded into an operator series. Thus

$$F(B) = \sum_{n=0}^{\infty} f_n B^n, \quad (1)$$

where  $f_n$  are constants. Also

$$\left[ \sum_i g_i G_i, \sum_j h_j H_j \right] = \sum_{i,j} g_i h_j [G_i, H_j], \quad (2)$$

where  $G_i$  and  $H_j$  are arbitrary operators and  $g_i$  and  $h_j$  arbitrary constants. Therefore,

$$[A, F(B)] = \sum_{n=0}^{\infty} f_n [A, B^n] = \sum_{n=0}^{\infty} f_n [A, B] n B^{n-1} = [A, B] F'(B) \quad (3)$$

follows if

$$[A, B^n] = [A, B] n B^{n-1}. \quad (4)$$

Thus we only need to prove the last equation which we will do by induction.

Step 1: For  $n = 0$ , equation (4) is true by inspection. For  $n = 1$ , it is again true by inspection. For  $n = 2$  (which is the first non-trivial case),

$$[A, B^2] = [A, B]B + B[A, B] = [A, B](2B), \quad (5)$$

where we have used the condition  $[B, [A, B]] = 0$ . Equation (5) satisfies equation (4) as required.

Step 2: Assume equation (4) for  $n - 1$ .

Step 3: For  $n$ , we find

$$\begin{aligned} [A, B^n] &= [A, B^{n-1}B] = [A, B^{n-1}]B + B^{n-1}[A, B] \\ &= [A, B](n-1)B^{n-2}B + [A, B]B^{n-1} = [A, B]nB^{n-1}, \end{aligned} \quad (6)$$

where we have used Step 2 and the condition  $[B, [A, B]] = 0$ .

We have now completed the prove of equation (4), and thus the proof of equation (3) which is the given identity.

b) Behold:

$$[x, p] = xp - px = xp - \frac{\hbar}{i} - xp = i\hbar .$$

c) From the part (b) answer  $[p, [x, p]] = [p, \hbar/i] = 0$ . Thus from the part (a) answer it follows that

$$[x, p^n] = [x, p]np^{n-1} = i\hbar np^{n-1} .$$

d) From the part (b) answer  $[x, [p, x]] = [x, -\hbar/i] = 0$ . Thus from the part (a) answer it follows that

$$[p, x^n] = [p, x]nx^{n-1} = -i\hbar nx^{n-1} .$$

**Redaction:** Jeffery, 2001jan01

008 qfull 01600 3 5 0 tough thinking: neutrino oscillation

**Extra keywords:** (Gr-120:3.58)

37. There are systems that exist apart from 3-dimensional Euclidean space: they are internal degrees of freedom such intrinsic spin of an electron or the proton-neutron identity of a nucleon (isospin: see, e.g., En-162 or Ga-429). Consider such an internal system for which we can only detect two states:

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

This internal system is 2-dimensional in the abstract vector sense of dimensional: i.e., it can be described completely by an orthonormal basis of consisting of the 2 vectors we have just given. When we measure this system we force it into one or other of these states: i.e., we make the fundamental perturbation. But the system can exist in a general state of course:

$$|\Psi(t)\rangle = c_+(t)|+\rangle + c_-(t)|-\rangle = \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix} .$$

- a) Given that  $|\Psi(t)\rangle$  is **NORMALIZED**, what equation must the coefficients  $c_+(t)$  and  $c_-(t)$  satisfy.
- b) For reasons only known to Mother Nature, the states we can measure (eigenvectors of whatever operator they may be)  $|+\rangle$  and  $|-\rangle$  are **NOT** eigenstates of the Hamiltonian that governs the time evolution of internal system. Let the Hamiltonian's eigenstates (i.e., the stationary states) be  $|+\prime\rangle$  and  $|-\prime\rangle$ : i.e.,

$$H|+\prime\rangle = E_+|+\prime\rangle \quad \text{and} \quad H|-\prime\rangle = E_-|-\prime\rangle ,$$

where  $E_+$  and  $E_-$  are the eigen-energies. Verify that the general state  $|\Psi(t)\rangle$  expanded in these energy eigenstates,

$$|\Psi(t)\rangle = c_+e^{-iE_+t/\hbar}|+\prime\rangle + c_-e^{-iE_-t/\hbar}|-\prime\rangle$$

satisfies the general vector form of the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H|\Psi(t)\rangle .$$

**HINT:** This requires a one-line answer.

- c) The Hamiltonian for this internal system has no differential operator form since there is no wave function. The matrix form in the  $|+\rangle$  and  $|-\rangle$  representation is

$$H = \begin{pmatrix} f & g \\ g & f \end{pmatrix} .$$

Given that  $H$  is Hermitian, prove that  $f$  and  $g$  must be real.

- d) Solve for the eigenvalues (i.e., eigen-energies) of Hamiltonian  $H$  and for its normalized eigenvectors  $|+\prime\rangle$  and  $|-\prime\rangle$  in column vector form.

e) Given at  $t = 0$  that

$$|\Psi(0)\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

show that

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}}(a+b)e^{-i(f+g)t/\hbar}|+\rangle + \frac{1}{\sqrt{2}}(a-b)e^{-i(f-g)t/\hbar}|-\rangle$$

and then show that

$$|\Psi(t)\rangle = e^{-ift/\hbar} \left[ a \begin{pmatrix} \cos(gt/\hbar) \\ -i \sin(gt/\hbar) \end{pmatrix} + b \begin{pmatrix} -i \sin(gt/\hbar) \\ \cos(gt/\hbar) \end{pmatrix} \right].$$

**HINT:** Recall the time-zero coefficients of expansion in basis  $\{|\phi_i\rangle\}$  are given by  $\langle\phi_i|\Psi(0)\rangle$ .

f) For the state found given the part (e) question, what is the probability at any time  $t$  of measuring (i.e., forcing by the fundamental perturbation) the system into state

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} ?$$

**HINT:** Note  $a$  and  $b$  are in general complex.

g) Set  $a = 1$  and  $b = 0$  in the probability expression found in the part (f) answer. What is the probability of measuring the system in state  $|+\rangle$ ? in state  $|-\rangle$ ? What is the system doing between the two states?

**NOTE:** The weird kind of oscillation between detectable states we have discussed is a simple model of neutrino oscillation. Just as an example, the detectable states could be the electron neutrino and muon neutrino and the particle oscillates between them. Really there are three flavors of neutrinos and a three-way oscillation may occur. There is growing evidence that neutrino oscillation does happen. (This note may be somewhat outdated due to that growth of evidence.)

**SUGGESTED ANSWER:**

a) Behold:

$$1 = \langle\Psi(t)|\Psi(t)\rangle = (c_+(t)^*, c_-(t)^*) \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix} = |c_+(t)|^2 + |c_-(t)|^2.$$

Thus  $c_+(t)$  and  $c_-(t)$  satisfy

$$1 = |c_+(t)|^2 + |c_-(t)|^2.$$

b) Behold:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle &= E_+ c_+ e^{-iE_+ t/\hbar} |+\rangle + E_- c_- e^{-iE_- t/\hbar} |-\rangle \\ &= c_+ e^{-iE_+ t/\hbar} H |+\rangle + c_- e^{-iE_- t/\hbar} H |-\rangle \\ &= H |\Psi(t)\rangle. \end{aligned}$$

c) Since  $H$  is Hermitian,  $H^\dagger = H$ . Therefore

$$\begin{pmatrix} f^* & g^* \\ g^* & f^* \end{pmatrix} = H^\dagger = H \begin{pmatrix} f & g \\ g & f \end{pmatrix}.$$

Thus  $f^* = f$  and  $g^* = g$ . Therefore  $f$  and  $g$  are real.

d) The eigenvalue equation is

$$(f - E)^2 - g^2 = 0$$

which by inspection has solutions

$$E_\pm = f \pm g.$$

The equation for the column vector elements is

$$f u_\pm + g v_\pm = (f \pm g) u_\pm$$

leading to

$$v_{\pm} = \pm u_{\pm} .$$

Thus the eigenvectors are given by

$$|\pm'\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} .$$

e) The time zero coefficients are given by

$$c_{\pm} = \frac{1}{\sqrt{2}}(1, \pm 1) \cdot \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{2}}(a \pm b) .$$

It immediately follows that

$$\begin{aligned} |\Psi(t)\rangle &= \frac{1}{\sqrt{2}}(a+b)e^{-i(f+g)t/\hbar}|+\rangle + \frac{1}{\sqrt{2}}(a-b)e^{-i(f-g)t/\hbar}|-\rangle \\ &= \frac{1}{\sqrt{2}}(a+b)e^{-i(f+g)t/\hbar} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{\sqrt{2}}(a-b)e^{-i(f-g)t/\hbar} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\ &= \frac{1}{2}ae^{-ift/\hbar} \begin{pmatrix} e^{-igt/\hbar} + e^{igt/\hbar} \\ e^{-igt/\hbar} - e^{igt/\hbar} \end{pmatrix} + \frac{1}{2}be^{-ift/\hbar} \begin{pmatrix} e^{-igt/\hbar} - e^{igt/\hbar} \\ e^{-igt/\hbar} + e^{igt/\hbar} \end{pmatrix} \\ &= e^{-ift/\hbar} \left[ a \begin{pmatrix} \cos(gt/\hbar) \\ -i \sin(gt/\hbar) \end{pmatrix} + b \begin{pmatrix} -i \sin(gt/\hbar) \\ \cos(gt/\hbar) \end{pmatrix} \right] . \end{aligned}$$

f) The amplitude for measuring the system in state  $|+\rangle$  is

$$\begin{aligned} \langle +|\Psi(t)\rangle &= (1, 0) \cdot e^{-ift/\hbar} \left[ a \begin{pmatrix} \cos(gt/\hbar) \\ -i \sin(gt/\hbar) \end{pmatrix} + b \begin{pmatrix} -i \sin(gt/\hbar) \\ \cos(gt/\hbar) \end{pmatrix} \right] \\ &= e^{-ift/\hbar} [a \cos(gt/\hbar) - ib \sin(gt/\hbar)] . \end{aligned}$$

Thus the probability is

$$\begin{aligned} |\langle +|\Psi(t)\rangle|^2 &= |a|^2 \cos^2(gt/\hbar) + |b|^2 \sin^2(gt/\hbar) + 2\text{Re}[a(-ib)^*] \cos(gt/\hbar) \sin(gt/\hbar) \\ &= |a|^2 \cos^2(gt/\hbar) + |b|^2 \sin^2(gt/\hbar) + 2\text{Re}[iab^*] \cos(gt/\hbar) \sin(gt/\hbar) \\ &= |a|^2 \cos^2(gt/\hbar) + |b|^2 \sin^2(gt/\hbar) - 2\text{Im}[ab^*] \cos(gt/\hbar) \sin(gt/\hbar) , \end{aligned}$$

where we have used the fact that

$$\text{Re}[iz] = \text{Re}[ix - y] = -y = -\text{Im}[z] .$$

If  $ab^*$  were pure real (which would be most easily arranged if  $a$  and  $b$  separately were pure real), the cross term would vanish.

g) If  $a = 1$  and  $b = 0$ , the probability of measuring the system in state  $|+\rangle$  is

$$|\langle +|\Psi(t)\rangle|^2 = \cos^2(gt/\hbar) .$$

The probability of measuring the system in state  $|-\rangle$  is

$$|\langle -|\Psi(t)\rangle|^2 = 1 - \cos^2(gt/\hbar) = \sin^2(gt/\hbar) .$$

The system is oscillating between the two states.

**Redaction:** Jeffery, 2001jan01



## Appendix 2 Quantum Mechanics Equation Sheet

**Note:** This equation sheet is intended for students writing tests or reviewing material. Therefore it neither intended to be complete nor completely explicit. There are fewer symbols than variables, and so some symbols must be used for different things.

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### 1 Constants not to High Accuracy

Constant Name	Symbol	Derived from CODATA 1998
Bohr radius	$a_{\text{Bohr}} = \frac{\lambda_{\text{Compton}}}{2\pi\alpha}$	$= 0.529 \text{ \AA}$
Boltzmann's constant	$k$	$= 0.8617 \times 10^{-6} \text{ eV K}^{-1}$ $= 1.381 \times 10^{-16} \text{ erg K}^{-1}$
Compton wavelength	$\lambda_{\text{Compton}} = \frac{h}{m_e c}$	$= 0.0246 \text{ \AA}$
Electron rest energy	$m_e c^2$	$= 5.11 \times 10^5 \text{ eV}$
Elementary charge squared	$e^2$	$= 14.40 \text{ eV \AA}$
Fine Structure constant	$\alpha = \frac{e^2}{\hbar c}$	$= 1/137.036$
Kinetic energy coefficient	$\frac{\hbar^2}{2m_e}$	$= 3.81 \text{ eV \AA}^2$
	$\frac{\hbar^2}{m_e}$	$= 7.62 \text{ eV \AA}^2$
Planck's constant	$h$	$= 4.15 \times 10^{-15} \text{ eV}$
Planck's h-bar	$\hbar$	$= 6.58 \times 10^{-16} \text{ eV}$
Rydberg Energy	$hc$	$= 12398.42 \text{ eV \AA}$
	$\hbar c$	$= 1973.27 \text{ eV \AA}$
	$E_{\text{Ryd}} = \frac{1}{2} m_e c^2 \alpha^2$	$= 13.606 \text{ eV}$

---

### 2 Some Useful Formulae

Leibniz's formula 
$$\frac{d^n(fg)}{dx^n} = \sum_{k=0}^n \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k} g}{dx^{n-k}}$$

Normalized Gaussian 
$$P = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x - \langle x \rangle)^2}{2\sigma^2}\right]$$

---

### 3 Schrödinger's Equation

$$H\Psi(x, t) = \left[ \frac{p^2}{2m} + V(x) \right] \Psi(x, t) = i\hbar \frac{\partial \Psi(x, t)}{\partial t}$$

$$H\psi(x) = \left[ \frac{p^2}{2m} + V(x) \right] \psi(x) = E\psi(x)$$

$$H\Psi(\vec{r}, t) = \left[ \frac{p^2}{2m} + V(\vec{r}) \right] \Psi(\vec{r}, t) = i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} \quad H|\Psi\rangle = i\hbar \frac{\partial}{\partial t} |\Psi\rangle$$

$$H\psi(\vec{r}) = \left[ \frac{p^2}{2m} + V(\vec{r}) \right] \psi(\vec{r}) = E\psi(\vec{r}) \quad H|\psi\rangle = E|\psi\rangle$$


---

#### 4 Some Operators

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

$$H = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

$$p = \frac{\hbar}{i} \nabla \quad p^2 = -\hbar^2 \nabla^2$$

$$H = \frac{p^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})$$

$$\nabla = \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} = \hat{r} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

#### 5 Kronecker Delta and Levi-Civita Symbol

$$\delta_{ij} = \begin{cases} 1, & i = j; \\ 0, & \text{otherwise} \end{cases} \quad \varepsilon_{ijk} = \begin{cases} 1, & ijk \text{ cyclic}; \\ -1, & ijk \text{ anticyclic}; \\ 0, & \text{if two indices the same.} \end{cases}$$

$$\varepsilon_{ijk} \varepsilon_{ilm} = \delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl} \quad (\text{Einstein summation on } i)$$

#### 6 Time Evolution Formulae

$$\text{General} \quad \frac{d\langle A \rangle}{dt} = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{\hbar} \langle i[H(t), A] \rangle$$

$$\text{Ehrenfest's Theorem} \quad \frac{d\langle \vec{r} \rangle}{dt} = \frac{1}{m} \langle \vec{p} \rangle \quad \text{and} \quad \frac{d\langle \vec{p} \rangle}{dt} = -\langle \nabla V(\vec{r}) \rangle$$

$$|\Psi(t)\rangle = \sum_j c_j(0) e^{-iE_j t/\hbar} |\phi_j\rangle$$

#### 7 Simple Harmonic Oscillator (SHO) Formulae

$$V(x) = \frac{1}{2} m \omega^2 x^2 \quad \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \right) \psi = E \psi$$

$$\beta = \sqrt{\frac{m\omega}{\hbar}} \quad \psi_n(x) = \frac{\beta^{1/2}}{\pi^{1/4}} \frac{1}{\sqrt{2^n n!}} H_n(\beta x) e^{-\beta^2 x^2/2} \quad E_n = \left( n + \frac{1}{2} \right) \hbar \omega$$

$$H_0(\beta x) = H_0(\xi) = 1 \quad H_1(\beta x) = H_1(\xi) = 2\xi$$

$$H_2(\beta x) = H_2(\xi) = 4\xi^2 - 2 \quad H_3(\beta x) = H_3(\xi) = 8\xi^3 - 12\xi$$

## 8 Position, Momentum, and Wavenumber Representations

$$p = \hbar k \quad E_{\text{kinetic}} = E_T = \frac{\hbar^2 k^2}{2m}$$

$$|\Psi(p, t)|^2 dp = |\Psi(k, t)|^2 dk \quad \Psi(p, t) = \frac{\Psi(k, t)}{\sqrt{\hbar}}$$

$$x_{\text{op}} = x \quad p_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad Q \left( x, \frac{\hbar}{i} \frac{\partial}{\partial x}, t \right) \quad \text{position representation}$$

$$x_{\text{op}} = -\frac{\hbar}{i} \frac{\partial}{\partial p} \quad p_{\text{op}} = p \quad Q \left( -\frac{\hbar}{i} \frac{\partial}{\partial p}, p, t \right) \quad \text{momentum representation}$$

$$\delta(x) = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{2\pi\hbar} dp \quad \delta(x) = \int_{-\infty}^{\infty} \frac{e^{ikx}}{2\pi} dk$$

$$\Psi(x, t) = \int_{-\infty}^{\infty} \Psi(p, t) \frac{e^{ipx/\hbar}}{(2\pi\hbar)^{1/2}} dp \quad \Psi(x, t) = \int_{-\infty}^{\infty} \Psi(k, t) \frac{e^{ikx}}{(2\pi)^{1/2}} dk$$

$$\Psi(p, t) = \int_{-\infty}^{\infty} \Psi(x, t) \frac{e^{-ipx/\hbar}}{(2\pi\hbar)^{1/2}} dx \quad \Psi(k, t) = \int_{-\infty}^{\infty} \Psi(x, t) \frac{e^{-ikx}}{(2\pi)^{1/2}} dx$$

$$\Psi(\vec{r}, t) = \int_{\text{all space}} \Psi(\vec{p}, t) \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}} d^3p \quad \Psi(\vec{r}, t) = \int_{\text{all space}} \Psi(\vec{k}, t) \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} d^3k$$

$$\Psi(\vec{p}, t) = \int_{\text{all space}} \Psi(\vec{r}, t) \frac{e^{-i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}} d^3r \quad \Psi(\vec{k}, t) = \int_{\text{all space}} \Psi(\vec{r}, t) \frac{e^{-i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} d^3r$$

## 9 Commutator Formulae

$$[A, BC] = [A, B]C + B[A, C] \quad \left[ \sum_i a_i A_i, \sum_j b_j B_j \right] = \sum_{i,j} a_i b_j [A_i, B_j]$$

$$\text{if } [B, [A, B]] = 0 \quad \text{then } [A, F(B)] = [A, B]F'(B)$$

$$[x, p] = i\hbar \quad [x, f(p)] = i\hbar f'(p) \quad [p, g(x)] = -i\hbar g'(x)$$

$$[a, a^\dagger] = 1 \quad [N, a] = -a \quad [N, a^\dagger] = a^\dagger$$

## 10 Uncertainty Relations and Inequalities

$$\sigma_x \sigma_p = \Delta x \Delta p \geq \frac{\hbar}{2} \quad \sigma_Q \sigma_Q = \Delta Q \Delta R \geq \frac{1}{2} |\langle i[Q, R] \rangle|$$

$$\sigma_H \Delta t_{\text{scale time}} = \Delta E \Delta t_{\text{scale time}} \geq \frac{\hbar}{2}$$

## 11 Probability Amplitudes and Probabilities

$$\Psi(x, t) = \langle x | \Psi(t) \rangle \quad P(dx) = |\Psi(x, t)|^2 dx \quad c_i(t) = \langle \phi_i | \Psi(t) \rangle \quad P(i) = |c_i(t)|^2$$

## 12 Spherical Harmonics

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \quad Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2} \cos(\theta) \quad Y_{1,\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin(\theta) e^{\pm i\phi}$$

$$L^2 Y_{\ell m} = \ell(\ell+1) \hbar^2 Y_{\ell m} \quad L_z Y_{\ell m} = m \hbar Y_{\ell m} \quad |m| \leq \ell \quad m = -\ell, -\ell+1, \dots, \ell-1, \ell$$

0	1	2	3	4	5	6	...
<i>s</i>	<i>p</i>	<i>d</i>	<i>f</i>	<i>g</i>	<i>h</i>	<i>i</i>	...

## 13 Hydrogenic Atom

$$\psi_{n\ell m} = R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \quad \ell \leq n-1 \quad \ell = 0, 1, 2, \dots, n-1$$

$$a_z = \frac{a}{Z} \left( \frac{m_e}{m_{\text{reduced}}} \right) \quad a_0 = \frac{\hbar}{m_e c \alpha} = \frac{\lambda_C}{2\pi\alpha} \quad \alpha = \frac{e^2}{\hbar c}$$

$$R_{10} = 2a_Z^{-3/2} e^{-r/a_Z} \quad R_{20} = \frac{1}{\sqrt{2}} a_Z^{-3/2} \left( 1 - \frac{1}{2} \frac{r}{a_Z} \right) e^{-r/(2a_Z)}$$

$$R_{21} = \frac{1}{\sqrt{24}} a_Z^{-3/2} \frac{r}{a_Z} e^{-r/(2a_Z)}$$

$$R_{n\ell} = - \left\{ \left( \frac{2}{na_Z} \right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3} \right\}^{1/2} e^{-\rho/2} \rho^\ell L_{n+\ell}^{2\ell+1}(\rho) \quad \rho = \frac{2r}{nr_Z}$$

$$L_q(x) = e^x \left( \frac{d}{dx} \right)^q (e^{-x} x^q) \quad \text{Rodrigues's formula for the Laguerre polynomials}$$

$$L_q^j(x) = \left( \frac{d}{dx} \right)^j L_q(x) \quad \text{Associated Laguerre polynomials}$$

$$\langle r \rangle_{n\ell m} = \frac{a_Z}{2} [3n^2 - \ell(\ell+1)]$$

$$\text{Nodes} = (n-1) - \ell \quad \text{not counting zero or infinity}$$

$$E_n = -\frac{1}{2}m_e c^2 \alpha^2 \frac{Z^2}{n^2} \frac{m_{\text{reduced}}}{m_e} = -E_{\text{Ryd}} \frac{Z^2}{n^2} \frac{m_{\text{reduced}}}{m_e} = -13.606 \frac{Z^2}{n^2} \frac{m_{\text{reduced}}}{m_e} \text{ eV}$$

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#### 14 General Angular Momentum Formulae

$$[J_i, J_j] = i\hbar \varepsilon_{ijk} J_k \quad (\text{Einstein summation on } k) \quad [J^2, \vec{J}] = 0$$

$$J^2 |jm\rangle = j(j+1)\hbar^2 |jm\rangle \quad J_z |jm\rangle = m\hbar |jm\rangle$$

$$J_{\pm} = J_x \pm iJ_y \quad J_{\pm} |jm\rangle = \hbar \sqrt{j(j+1) - m(m \pm 1)} |jm \pm 1\rangle$$

$$J_{\left\{ \begin{smallmatrix} x \\ y \end{smallmatrix} \right\}} = \left\{ \begin{smallmatrix} \frac{1}{2} \\ \frac{1}{2i} \end{smallmatrix} \right\} (J_+ \pm J_-) \quad J_{\pm}^{\dagger} J_{\pm} = J_{\mp} J_{\pm} = J^2 - J_z (J_z \pm \hbar)$$

$$[J_{fi}, J_{gj}] = \delta_{fg} i\hbar \varepsilon_{ijk} J_k \quad \vec{J} = \vec{J}_1 + \vec{J}_2 \quad J^2 = J_1^2 + J_2^2 + J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z}$$

$$J_{\pm} = J_{1\pm} + J_{2\pm} \quad |j_1 j_2 j m\rangle = \sum_{m_1 m_2, m=m_1+m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle |j_1 j_2 j m\rangle$$

$$|j_1 - j_2| \leq j \leq j_1 + j_2 \quad \sum_{|j_1 - j_2|}^{j_1 + j_2} (2j + 1) = (2j_1 + 1)(2j_2 + 1)$$

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#### 15 Spin 1/2 Formulae

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$|\pm\rangle_x = \frac{1}{\sqrt{2}} (|+\rangle \pm |-\rangle) \quad |\pm\rangle_y = \frac{1}{\sqrt{2}} (|+\rangle \pm i|-\rangle) \quad |\pm\rangle_z = |\pm\rangle$$

$$|++\rangle = |1, +\rangle |2, +\rangle \quad |+-\rangle = \frac{1}{\sqrt{2}} (|1, +\rangle |2, -\rangle \pm |1, -\rangle |2, +\rangle) \quad |--\rangle = |1, -\rangle |2, -\rangle$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk} \sigma_k \quad [\sigma_i, \sigma_j] = 2i\varepsilon_{ijk} \sigma_k \quad \{\sigma_i, \sigma_j\} = 2\delta_{ij}$$

$$(\vec{A} \cdot \vec{\sigma})(\vec{B} \cdot \vec{\sigma}) = \vec{A} \cdot \vec{B} + i(\vec{A} \times \vec{B}) \cdot \vec{\sigma}$$

$$\frac{d(\vec{S} \cdot \hat{n})}{d\alpha} = -\frac{i}{\hbar} [\vec{S} \cdot \hat{\alpha}, \vec{S} \cdot \hat{n}] \quad \vec{S} \cdot \hat{n} = e^{-i\vec{S} \cdot \hat{\alpha}} \vec{S} \cdot \hat{n}_0 e^{i\vec{S} \cdot \hat{\alpha}} \quad |\hat{n}_{\pm}\rangle = e^{-i\vec{S} \cdot \hat{\alpha}} |\hat{z}_{\pm}\rangle$$

$$e^{ixA} = \mathbf{1} \cos(x) + iA \sin(x) \quad \text{if } A^2 = \mathbf{1} \quad e^{-i\vec{\sigma} \cdot \vec{\alpha}/2} = \mathbf{1} \cos(x) - i\vec{\sigma} \cdot \hat{\alpha} \sin(x)$$

$$\sigma_i f(\sigma_j) = f(\sigma_j) \sigma_i \delta_{ij} + f(-\sigma_j) \sigma_i (1 - \delta_{ij})$$

$$\mu_{\text{Bohr}} = \frac{e\hbar}{2m} = 0.927400915(23) \times 10^{-24} \text{ J/T} = 5.7883817555(79) \times 10^{-5} \text{ eV/T}$$

$$g = 2 \left( 1 + \frac{\alpha}{2\pi} + \dots \right) = 2.0023193043622(15)$$

$$\vec{\mu}_{\text{orbital}} = -\mu_{\text{Bohr}} \frac{\vec{L}}{\hbar} \quad \vec{\mu}_{\text{spin}} = -g\mu_{\text{Bohr}} \frac{\vec{S}}{\hbar} \quad \vec{\mu}_{\text{total}} = \vec{\mu}_{\text{orbital}} + \vec{\mu}_{\text{spin}} = -\mu_{\text{Bohr}} \frac{(\vec{L} + g\vec{S})}{\hbar}$$

$$H_{\mu} = -\vec{\mu} \cdot \vec{B} \quad H_{\mu} = \mu_{\text{Bohr}} B_z \frac{(L_z + gS_z)}{\hbar}$$

## 16 Time-Independent Approximation Methods

$$H = H^{(0)} + \lambda H^{(1)} \quad |\psi\rangle = N(\lambda) \sum_{k=0}^{\infty} \lambda^k |\psi_n^{(k)}\rangle$$

$$H^{(1)} |\psi_n^{(m-1)}\rangle (1 - \delta_{m,0}) + H^{(0)} |\psi_n^{(m)}\rangle = \sum_{\ell=0}^m E^{(m-\ell)} |\psi_n^{(\ell)}\rangle \quad |\psi_n^{(\ell>0)}\rangle = \sum_{m=0, m \neq n}^{\infty} a_{nm} |\psi_n^{(0)}\rangle$$

$$|\psi_n^{1\text{st}}\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{\text{all } k, k \neq n} \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} |\psi_k^{(0)}\rangle$$

$$E_n^{1\text{st}} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle$$

$$E_n^{2\text{nd}} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle + \lambda^2 \sum_{\text{all } k, k \neq n} \frac{|\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$E(\phi) = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} \quad \delta E(\phi) = 0$$

$$H_{kj} = \langle \phi_k | H | \phi_j \rangle \quad H\vec{c} = E\vec{c}$$

## 17 Time-Dependent Perturbation Theory

$$\pi = \int_{-\infty}^{\infty} \frac{\sin^2(x)}{x^2} dx$$

$$\Gamma_{0 \rightarrow n} = \frac{2\pi}{\hbar} |\langle n | H_{\text{perturbation}} | 0 \rangle|^2 \delta(E_n - E_0)$$

## 18 Interaction of Radiation and Matter

$$\vec{E}_{\text{op}} = -\frac{1}{c} \frac{\partial \vec{A}_{\text{op}}}{\partial t} \quad \vec{B}_{\text{op}} = \nabla \times \vec{A}_{\text{op}}$$

## 19 Box Quantization

$$kL = 2\pi n, \quad n = 0, \pm 1, \pm 2, \dots \quad k = \frac{2\pi n}{L} \quad \Delta k_{\text{cell}} = \frac{2\pi}{L} \quad \Delta k_{\text{cell}}^3 = \frac{(2\pi)^3}{V}$$

$$dN_{\text{states}} = g \frac{k^2 dk d\Omega}{(2\pi)^3 / V}$$

## 20 Identical Particles

$$|a, b\rangle = \frac{1}{\sqrt{2}} (|1, a; 2, b\rangle \pm |1, b; 2, a\rangle)$$

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \pm \psi_b(\vec{r}_1)\psi_a(\vec{r}_2))$$

## 21 Second Quantization

$$[a_i, a_j^\dagger] = \delta_{ij} \quad [a_i, a_j] = 0 \quad [a_i^\dagger, a_j^\dagger] = 0 \quad |N_1, \dots, N_n\rangle = \frac{(a_n^\dagger)^{N_n}}{\sqrt{N_n!}} \dots \frac{(a_1^\dagger)^{N_1}}{\sqrt{N_1!}} |0\rangle$$

$$\{a_i, a_j^\dagger\} = \delta_{ij} \quad \{a_i, a_j\} = 0 \quad \{a_i^\dagger, a_j^\dagger\} = 0 \quad |N_1, \dots, N_n\rangle = (a_n^\dagger)^{N_n} \dots (a_1^\dagger)^{N_1} |0\rangle$$

$$\Psi_s(\vec{r})^\dagger = \sum_{\vec{p}} \frac{e^{-i\vec{p}\cdot\vec{r}}}{\sqrt{V}} a_{\vec{p}s}^\dagger \quad \Psi_s(\vec{r}) = \sum_{\vec{p}} \frac{e^{i\vec{p}\cdot\vec{r}}}{\sqrt{V}} a_{\vec{p}s}$$

$$[\Psi_s(\vec{r}), \Psi_{s'}(\vec{r}')]_{\mp} = 0 \quad [\Psi_s(\vec{r})^\dagger, \Psi_{s'}(\vec{r}')^\dagger]_{\mp} = 0 \quad [\Psi_s(\vec{r}), \Psi_{s'}(\vec{r}')^\dagger]_{\mp} = \delta(\vec{r} - \vec{r}') \delta_{ss'}$$

$$|\vec{r}_1 s_1, \dots, \vec{r}_n s_n\rangle = \frac{1}{\sqrt{n!}} \Psi_{s_n}(\vec{r}_n)^\dagger \dots \Psi_{s_1}(\vec{r}_1)^\dagger |0\rangle$$

$$\Psi_s(\vec{r})^\dagger |\vec{r}_1 s_1, \dots, \vec{r}_n s_n\rangle \sqrt{n+1} |\vec{r}_1 s_1, \dots, \vec{r}_n s_n, \vec{r}s\rangle$$

$$|\Phi\rangle = \int d\vec{r}_1 \dots d\vec{r}_n \Phi(\vec{r}_1, \dots, \vec{r}_n) |\vec{r}_1 s_1, \dots, \vec{r}_n s_n\rangle$$

$$1_n = \sum_{s_1 \dots s_n} \int d\vec{r}_1 \dots d\vec{r}_n |\vec{r}_1 s_1, \dots, \vec{r}_n s_n\rangle \langle \vec{r}_1 s_1, \dots, \vec{r}_n s_n| \quad 1 = |0\rangle \langle 0| + \sum_{n=1}^{\infty} 1_n$$

$$N = \sum_{\vec{p}s} a_{\vec{p}s}^\dagger a_{\vec{p}s} \quad T = \sum_{\vec{p}s} \frac{p^2}{2m} a_{\vec{p}s}^\dagger a_{\vec{p}s}$$

$$\rho_s(\vec{r}) = \Psi_s(\vec{r})^\dagger \Psi_s(\vec{r}) \quad N = \sum_s \int d\vec{r} \rho_s(\vec{r}) \quad T = \frac{1}{2m} \sum_s \int d\vec{r} \nabla \Psi_s(\vec{r})^\dagger \cdot \nabla \Psi_s(\vec{r})$$

$$\vec{j}_s(\vec{r}) = \frac{1}{2im} [\Psi_s(\vec{r})^\dagger \nabla \Psi_s(\vec{r}) - \Psi_s(\vec{r}) \nabla \Psi_s(\vec{r})^\dagger]$$

$$G_s(\vec{r} - \vec{r}') = \frac{3n \sin(x) - x \cos(x)}{2x^3} \quad g_{ss'}(\vec{r} - \vec{r}') = 1 - \delta_{ss'} \frac{G_s(\vec{r} - \vec{r}')^2}{(n/2)^2}$$

$$v_{2\text{nd}} = \frac{1}{2} \sum_{ss'} \int d\vec{r} d\vec{r}' v(\vec{r} - \vec{r}') \Psi_s(\vec{r})^\dagger \Psi_{s'}(\vec{r}')^\dagger \Psi_{s'}(\vec{r}') \Psi_s(\vec{r})$$

$$v_{2\text{nd}} = \frac{1}{2V} \sum_{pp'qq'} \sum_{ss'} v_{\vec{p}-\vec{p}'} \delta_{\vec{p}+\vec{q}, \vec{p}'+\vec{q}'} a_{\vec{p}s}^\dagger a_{\vec{q}s'}^\dagger a_{\vec{q}'s'} a_{\vec{p}'s} \quad v_{\vec{p}-\vec{p}'} = \int d\vec{r} e^{-i(\vec{p}-\vec{p}') \cdot \vec{r}} v(\vec{r})$$

## 22 Klein-Gordon Equation

$$E = \sqrt{p^2 c^2 + m^2 c^4} \quad \frac{1}{c^2} \left( i\hbar \frac{\partial}{\partial t} \right)^2 \Psi(\vec{r}, t) = \left[ \left( \frac{\hbar}{i} \nabla \right)^2 + m^2 c^2 \right] \Psi(\vec{r}, t)$$

$$\left[ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \left( \frac{mc}{\hbar} \right)^2 \right] \Psi(\vec{r}, t) = 0$$

$$\rho = \frac{i\hbar}{2mc^2} \left( \Psi^* \frac{\partial \Psi}{\partial t} - \Psi \frac{\partial \Psi^*}{\partial t} \right) \quad \vec{j} = \frac{\hbar}{2im} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*)$$

$$\frac{1}{c^2} \left( i\hbar \frac{\partial}{\partial t} - e\Phi \right)^2 \Psi(\vec{r}, t) = \left[ \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A} \right)^2 + m^2 c^2 \right] \Psi(\vec{r}, t)$$

$$\Psi_+(\vec{p}, E) = e^{i(\vec{p} \cdot \vec{r} - Et)/\hbar} \quad \Psi_-(\vec{p}, E) = e^{-i(\vec{p} \cdot \vec{r} - Et)/\hbar}$$