

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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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.
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
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.
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) $U^{-1} = U^*$.

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.
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.
 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 $|-\alpha\rangle$ such that

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

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

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

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 $h \neq 0$.
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.
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.

- Write down the general step of the Gram-Schmidt procedure.
- Why must an orthonormal set of non-null vectors be a linearly independent.
- 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 $|\alpha_a\rangle$?
- 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?
- 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.
- 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.
- 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.

- 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 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 correspondence. **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?

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

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

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

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

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 2×2 unit matrices.

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.

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.,

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

and

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

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.

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.

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

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

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

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.

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
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) $\langle f|(-i)|g\rangle$.
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
23. Given general operators A and B , $(AB)^\dagger$ equals:
a) AB . b) $A^\dagger B^\dagger$. c) A . d) B . e) $B^\dagger A^\dagger$.
24. The Hermitian conjugate of the operator $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A$ (with λ 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) $A^\dagger|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda^*$.
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.
26. The parity operator Π acting on $f(x)$ gives:
 df/dx . b) $1/f(x)$. c) $f(-x)$. d) 0. e) a spherical harmonic.
27. Given the position representation for an expectation value

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

what is the bracket 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) $\langle Q|\Psi|Q\rangle$.
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.
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
30. In the precisely-formulated time-energy inequality, the Δt 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.
31. The statements “two observables commute” and “a common eigenset can be constructed for two observables” are
- 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.
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)?

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.

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?

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?

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

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

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

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.)

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.

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

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

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

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

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

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

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

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

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

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

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

14 General Angular Momentum Formulae

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

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

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

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

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

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

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

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

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

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

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

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

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