NPTEL COURSE ON QUANTUM PHYSICS

V. Balakrishnan
Department of Physics, Indian Institute of Technology Madras
Chennai 600 036, India

Some mathematical preliminaries: Linear vector spaces

There are many textbooks and monographs that give excellent accounts of the mathematics required for quantum mechanics, at different levels of sophistication. Here are just a few of these references (google for their publication details!):

N. I. Akhiezer and I. M. Glazman, *Theory of Linear Operators in Hilbert Space*
R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Vol. 1
P. Dennery and A. Krzywicki, *Mathematics for Physicists*
P. A. M. Dirac, *Principles of Quantum Mechanics*
B. Friedman, *Principles and Techniques of Applied Mathematics*
P. R. Halmos, *Finite Dimensional Vector Spaces*
T. F. Jordan, *Linear Operators for Quantum Mechanics*
D. W. Lewis, *Matrix Theory*

A **linear vector space** (or LVS) $\mathbb{V}$ is a set of elements $|\psi\rangle, |\phi\rangle, \ldots$ called **vectors**, with an operation called **addition** satisfying the following properties:

(i) $|\phi\rangle + |\psi\rangle = |\psi\rangle + |\phi\rangle \in \mathbb{V}\,,\ \forall\, |\phi\rangle\,,\ |\psi\rangle \in \mathbb{V}$

(ii) $|\phi\rangle + (|\psi\rangle + |\chi\rangle) = (|\phi\rangle + |\psi\rangle) + |\chi\rangle$

(iii) $\exists$ a unique null vector $|\Omega\rangle \in \mathbb{V}$ such that $|\phi\rangle + |\Omega\rangle = |\phi\rangle\,,\ \forall\, |\phi\rangle \in \mathbb{V}$

(iv) $\exists$ a unique vector $-|\phi\rangle \in \mathbb{V}$ for every $|\phi\rangle$ such that $|\phi\rangle + (-|\phi\rangle) = |\Omega\rangle\,.$

There is also an operation of **multiplication by scalars** $a, b, \ldots$ belonging to $\mathbb{R}$ (the field of real numbers) or $\mathbb{C}$ (the field of complex numbers), such that

(v) $a\,|\phi\rangle \in \mathbb{V}\,,\ \ \forall a \in \mathbb{R}$ or $\mathbb{C}$ and $|\phi\rangle \in \mathbb{V}$

(vi) $a\,(b\,|\psi\rangle) = (ab)\,|\psi\rangle$

(vii) $a\,(|\psi\rangle + |\phi\rangle) = a\,|\psi\rangle + a\,|\phi\rangle$

(viiii) $(a+b)\,|\psi\rangle = a\,|\psi\rangle + b\,|\psi\rangle$

(ix) $1\,|\psi\rangle = |\psi\rangle$

(x) $0\,|\psi\rangle = 0\,.$ It is because of this property that we may as well use the usual symbol 0 for both the null vector $|\Omega\rangle$ and for the usual scalar zero.

If the scalars $a, b, \ldots$ are restricted to the real numbers, the LVS is a 'real LVS'; if the scalars are complex numbers, we have a 'complex LVS'.[1]

The dual space: Every LVS has a **dual** that is also an LVS. The notation used for the elements of this dual LVS is $\langle\phi|\,, \langle\psi|\,\ldots.$ The inner product $\langle\phi|\psi\rangle$ has the general properties

[1]The scalars may also be drawn from fields other than the real or complex number fields, but we shall not consider these generalizations.

(i) $\langle\phi|(|\psi\rangle + |\chi\rangle) = \langle\phi|\psi\rangle + \langle\phi|\chi\rangle$

(ii) $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$

(iii) $\langle\phi|a\,\psi\rangle = a\langle\phi|\psi\rangle$

(iv) $\langle a\,\phi|\psi\rangle = a^*\langle\phi|\psi\rangle$

The norm of a vector is given by $\| \psi \| = \langle\psi|\psi\rangle^{1/2}$. The norm is positive definite for every non-null vector. It vanishes if and only if $|\psi\rangle = |\Omega\rangle$.

A basis in the LVS is a set of vectors that (i) are linearly independent and (ii) span the space. A basis has n vectors if and only if the dimensionality of the LVS is n. Every n-dimensional LVS is isomorphic to the Euclidean LVS $\mathbb{R}^n$.

An **infinite-dimensional LVS** is one that has no n-dimensional basis for any positive integer n.

Orthonormal basis: Given a basis set, we can make it an orthonormal basis by the **Gram-Schmidt orthonormalization procedure**. If the set of vectors $\{|\phi_j\rangle\}$ is an orthonormal basis, we have the relations

$$\langle\phi_j|\phi_k\rangle = \delta_{jk} \quad (\textbf{orthonormality})$$

and

$$\sum_j |\phi_j\rangle\langle\phi_j| = I, \quad (\textbf{completeness})$$

where I is the unit operator in the LVS. It follows that any vector $|\psi\rangle$ in the LVS can be uniquely expanded in terms of the basis according to

$$|\psi\rangle = \sum_j c_j\,|\phi_j\rangle, \quad \text{where} \quad c_j = \langle\phi_j\,|\psi\rangle.$$

'Uniquely expanded' means that the coefficients c_j uniquely determine $|\psi\rangle$, and vice versa.

Change of basis: The basis set in any LVS is by no means unique, although its dimensionality is. Given two orthonormal basis sets $\{|\phi_j\rangle\}$ and $\{|\chi_k\rangle\}$, we have the expansions

$$|\psi\rangle = \sum_j c_j\,|\phi_j\rangle = \sum_k d_k\,|\chi_k\rangle\,,$$

for any vector $|\psi\rangle$. The expansion coefficients $c_j = \langle\phi_j\,|\psi\rangle$ and $d_k = \langle\chi_k\,|\psi\rangle$ are related by

$$c_j = \sum_k d_k\,\langle\phi_j\,|\chi_k\rangle, \quad d_k = \sum_j c_j\,\langle\chi_k\,|\phi_j\rangle.$$

1. Check whether the following sets of elements form an LVS. If they do, find the dimensionality of the LVS.

(a) The set of all $n \times n$ matrices with complex entries.

(b) The set of all polynomials (of all orders) of a complex variable z.

(c) The set of all (Cartesian) tensors of rank 2 in three dimensions.

(d) The set of all antisymmetric (Cartesian) tensors of rank 2 in three dimensions.

(e) The set of all 2×2 matrices whose trace is zero.

(f) The set of all solutions of the differential equation $\dfrac{d^2y}{dx^2} - 3\dfrac{dy}{dx} + 2y = 0$.

(g) The set of all $n \times n$ unitary matrices. (U is unitary iff $U^\dagger U = UU^\dagger = I$.)

(h) The set of all $n \times n$ hermitian matrices (with multiplication by real scalars).

2. In the three-dimensional LVS with basis vectors

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |\phi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

find a vector $|\psi\rangle$ such that $\langle\phi_i\,|\psi\rangle = 1$ for $i = 1, 2$ and 3.

3. In a three-dimensional LVS, consider the three vectors

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad |\psi_2\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad |\psi_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}.$$

(a) Show that they are linearly independent.

(b) Use the Gram-Schmidt procedure to construct an orthonormal basis $\{|\phi_i\rangle\}$ from these three vectors.

4. The Cauchy-Schwarz inequality is of fundamental importance. It says that

$$|\langle\phi\,|\psi\rangle| \leq \| \phi \| \, \| \psi \|,$$

the equality holding if and only if $|\phi\rangle$ and $|\psi\rangle$ are linearly dependent. In terms of ordinary vectors in Euclidean space, it amounts to saying that the cosine of the angle between two vectors has a magnitude between 0 and 1, the limiting value of unity occurring if and only if the vectors are collinear. Establish the Cauchy-Schwarz inequality.

Hint: Consider the inner product $\langle\phi + a\,\psi\,|\,\phi + a\,\psi\rangle$ where $|\phi\rangle$, $|\psi\rangle \in \mathbb{V}$, and a is an arbitrary complex number. Choosing a appropriately leads to the desired inequality.

5. The triangle inequality: Use the Cauchy-Schwarz inequality to establish the triangle inequality (or Minkowski inequality)

$$\| \phi + \psi \| \leq \| \phi \| + \| \psi \|$$

for any two vectors $|\phi\rangle$ and $|\psi\rangle \in \mathbb{V}$.

6. Here are a couple of useful results:

(a) Let $|\psi\rangle$ and $|\phi\rangle$ be two linearly independent vectors in a *real* LVS. Find the value of the (real) scalar α that makes $\| \psi - \alpha\,\phi \|$ a minimum.

(b) Same problem, in a *complex* LVS. (Note that any complex number α and its complex conjugate α^* are linearly independent!)

7. Show that the 2×2 unit matrix I and the three Pauli matrices, namely,

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

form a basis in the LVS of all 2×2 matrices. What is the corresponding basis if we restrict ourselves to the set of all *traceless* 2×2 matrices?

8. Which of the following infinite sequences $(x_1, x_2, \cdots)$ listed below belong to ℓ_2, the LVS of square-summable sequences?

(a) $x_n = (-1)^n \, (\ln n)/n$

(b) $x_n = n!/(2n)!$

(c) $x_n = (2/n)^n$

(d) $x_n = (2n+1)/(3n+4)^2$

(e) $x_n = e^n/n^n$

(f) $x_n = 2^{-n/2}$.

9. Identify the functions that belong to $\mathcal{L}_2(-\infty\,,\,\infty)$, the LVS of square-integrable functions of a real variable $x \in (-\infty, \infty)$.

(a) $f(x) = (x^2+1)^{-1/4}$

(b) $f(x) = e^{-x} \, \cos \, x$

(c) $f(x) = e^{-1/x^2}$

(d) $f(x) = (\sin \, x)/x$

(e) $f(x) = x^3 \, e^{-x^2}$

(f) $f(x) = (\tanh \, x)/x$.

10. In an n-dimensional LVS, consider the vectors $|\phi_k\rangle$ $(k = 1, 2, \ldots, n)$ given by

$$|\phi_1\rangle = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \end{pmatrix}^{\mathrm{T}}, \quad |\phi_2\rangle = \left(\frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}} \quad 0 \quad \cdots \quad 0 \right)^{\mathrm{T}}, \cdots\cdots,$$

$$|\phi_n\rangle = \left(\frac{1}{\sqrt{n}} \quad \frac{1}{\sqrt{n}} \quad \frac{1}{\sqrt{n}} \quad \cdots \quad \frac{1}{\sqrt{n}} \right)^{\mathrm{T}},$$

where the superscript T denotes the transpose. Construct a vector $|\psi\rangle$ such that $\langle \phi_k \, | \psi \rangle = 1$ for every $k \, (1 \le k \le n)$.

11. The set of all $n \times n$ matrices (with complex entries) forms an LVS. The inner product of two elements in this space may be *defined* as

$$(A,\, B) \stackrel{\text{def.}}{=} \mathrm{Tr} \, (A^\dagger B),$$

where $A^\dagger$ is the hermitian conjugate of A, and Tr denotes the trace.

(a) If A is hermitian, show that

$$(A,\, A) \, \ge \, \frac{1}{n} \, (I,\, A)^2.$$

(b) If A is an arbitrary $n \times n$ matrix, and U is an unitary $n \times n$ matrix, show that

$$(A,\, A) \, \ge \, \frac{1}{n} \, |(U^\dagger,\, A)|^2.$$

Operators on a linear space

Matrices as operators in an LVS: We may view $(n \times n)$ matrices as the representations of operators in an n-dimensional LVS. Every n-dimensional LVS is isomorphic to n-dimensional Euclidean space. The natural basis in this space is given by the ket vectors *represented* by the column matrices

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \ \cdots, \ |\phi_n\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}.$$

This space is self-dual. The natural basis in the dual space are the bra vectors $\langle\phi_i|$ represented by the row matrices that are the hermitian conjugates of the column matrices above. It is then easy to see that the *operator* $|\phi_i\rangle\langle\phi_j|$ is represented by a matrix whose ij^{th} element is unity, all its other elements being zero. In other words, any *matrix* A with elements a_{ij} can be regarded as the *representation* of an abstract *operator* A given by

$$\mathsf{A} = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \, |\phi_i\rangle\langle\phi_j|.$$

Thus the n^2 operators $|\phi_i\rangle\langle\phi_j|$ (where $i\,, j = 1, 2, \ldots, n$) comprise the **natural basis** for all *operators* acting on the vectors of the LVS. The orthonormality of the natural basis immediately yields

$$a_{ij} = \langle\phi_i|\mathsf{A}|\phi_j\rangle.$$

This is why an object like $\langle\phi_i|\mathsf{A}|\phi_j\rangle$ is called (what else!) a **matrix element** in quantum mechanics, even when the LVS is infinite-dimensional, and even when the basis set itself is a *non*denumerable basis or a **continuous basis**. We shall exploit this fact to use the same symbol for both the abstract operator as well as its matrix representation—e. g., we shall write A for both A and the matrix representing it (in the natural basis, unless otherwise specified). Which of the two is meant will be clear from the context.

Many of the definitions that follow below are obvious in the case of finite-dimensional vector spaces. It is the case of infinite-dimensional spaces that is non-trivial, and in which care must be exercised.

The domain of an operator: Let $\mathbb{V}$ denote a linear vector space. Then the **domain** $\mathbb{D}_A$ of the operator A is the subset of $\mathbb{V}$ such that the operator A acting on each element $|\phi\rangle \in \mathbb{D}$ yields an element $A|\phi\rangle = |\psi\rangle \in \mathbb{V}$.

The range of an operator: The set Δ_A consisting of elements $|\psi\rangle$, as $|\phi\rangle$ runs through all the elements of $\mathbb{D}$, is called the **range** of the operator A.

The inverse of an operator: If A maps each pair of different elements of $\mathbb{D}_A$ into a pair of different elements of Δ_A, then A has an **inverse** A^{-1} which maps the elements of Δ_A into the elements of $\mathbb{D}_A$. We then have

$$A^{-1}|\psi\rangle = |\phi\rangle \quad \text{if and only if} \quad A|\phi\rangle = |\psi\rangle.$$

Equality of operators: Two operators are equal if they have the same domain, and if they have the same action on each given vector in their common domain.

Linear manifolds: A subset $\mathbb{U}$ of $\mathbb{V}$ is a **linear manifold** if the following property is satisfied: given any pair of elements $|\phi\rangle, |\chi\rangle \in \mathbb{U}$, any arbitrary linear combination $\alpha|\phi\rangle + \beta|\chi\rangle$ (where α and β are scalars) is also an element of $\mathbb{U}$.

Cauchy sequences of operators and complete vector spaces: Recall that a sequence of complex numbers z_n is a **Cauchy sequence** if $|z_n - z_m| \to 0$ when both n and m tend to ∞. A Cauchy sequence is guaranteed to converge to a limit, i. e., $\lim_{n\to\infty} z_n$ exists, and is some complex number. A set that contains all its limit points is called a **closed set**.

In the same way, we can speak of sequences of vectors in an LVS. Such a sequence of vectors, say $\{|\phi_n\rangle\}$, is a Cauchy sequence if $\lim_{n,m\to\infty} \|\phi_n - \phi_m\| = 0$. Every Cauchy sequence of vectors converges to some limiting vector, i. e., $\lim_{n\to\infty} |\phi_n\rangle$ exists. If the limit vectors of all the Cauchy sequences of an LVS $\mathbb{V}$ also lie in $\mathbb{V}$, then $\mathbb{V}$ is said to be a **complete** LVS. *Every finite-dimensional LVS is complete.*

Subspaces: A linear manifold $\mathbb{U}$ in an LVS $\mathbb{V}$ is a **subspace** of the LVS if it is complete: that is, all Cauchy sequences of vectors belonging to $\mathbb{U}$ also lie in $\mathbb{U}$.

It turns out that it is easy to test whether a subset $\mathbb{U}$ of vectors in an LVS $\mathbb{V}$ is a subspace or not. All that is needed for this to be so is the following: (i) $\mathbb{U}$ must contain the null vector; (ii) the sum of any two vectors in $\mathbb{U}$ must lie in $\mathbb{U}$; (iii) any scalar multiple of any vector in $\mathbb{U}$ must lie in $\mathbb{U}$. A subspace of an LVS is also an LVS, with the same operations of addition and scalar multiplication as the original LVS.

Hilbert spaces are of primary importance in quantum mechanics: the state vector of a quantum mechanical system is a vector in some Hilbert space. A **Hilbert space** is a linear vector space that

(i) is complete, and
(ii) is equipped with an inner product.

A **separable Hilbert space** is one that has a *countable* or denumerable basis, finite or infinite (as opposed to an LVS that has no countable basis, but only non-denumerable basis sets). We shall only be concerned with separable Hilbert spaces.

Dimensionality of subspaces: If $\mathbb{U}_1$ and $\mathbb{U}_2$ are subspaces of an LVS, then so are their sum $(\mathbb{U}_1 + \mathbb{U}_2)$ and intersection $(\mathbb{U}_1 \cap \mathbb{U}_2)$. The dimensionalities of these subspaces are related by

$$\dim(\mathbb{U}_1 \cap \mathbb{U}_2) = \dim \mathbb{U}_1 + \dim \mathbb{U}_2 - \dim(\mathbb{U}_1 + \mathbb{U}_2).$$

Linear operators: A is a **linear operator** acting on the vectors of an LVS if

(i) $\mathbb{D}_A$ is a linear manifold, and
(ii) $A(\alpha|\phi\rangle + \beta|\chi\rangle) = \alpha A|\phi\rangle + \beta A|\chi\rangle$ for any scalars α and β.

Combinations of operators: If A and B are linear operators in $\mathbb{V}$, then any linear combination $C = aA + bB$ (where a and b are scalars) is also a linear operator with domain $\mathbb{D}_C = \mathbb{D}_A \cap \mathbb{D}_B$. The operators AB and BA are also linear operators. If A and B are bounded linear operators in all of $\mathbb{V}$, then so are AB and BA.

The adjoint of an operator: Let A be an operator A acting on the vectors of a linear space $\mathbb{V}$. Let (χ, ψ) denote the inner product in $\mathbb{V}$, i.e., $(\chi, \psi) \equiv \langle\chi|\psi\rangle$. If, for every pair of vectors $|\psi\rangle$ and $|\chi\rangle$ in $\mathbb{V}$, there is an operator B such that

$$(\chi\,,\, A\psi) = (B\chi\,,\, \psi),$$

then the operator B is the **adjoint** of the operator A, and will be denoted by $A^\dagger$. Thus the adjoint of the equation

$$A\,|\psi\rangle = |\phi\rangle \quad \text{is} \quad \langle\psi|\,A^\dagger = \langle\phi|.$$

It is easy to see that in the case of a finite-dimensional LVS of n dimensions, in which operators are representable by $(n \times n)$ matrices, the adjoint $A^\dagger$ is simply the hermitian conjugate (i.e., complex conjugate transpose) of the matrix A.

Self-adjoint operators: An operator A is **self-adjoint** if $A = A^\dagger$. For operators represented by (finite-dimensional) matrices, it is trivial to verify whether A is self-adjoint or not. In more general cases, we must not only ensure that the operator $A^\dagger$ as identified from the relation $(\chi\,,\, A\psi) = (A^\dagger\chi\,,\, \psi)$ is the same as the operator A, but *also* that $\mathbb{D}_A = \mathbb{D}_{A^\dagger}$. Only then can we assert that $A = A^\dagger$, i.e., that A is self-adjoint.

In general, it turns out that $\mathbb{D}_{A^\dagger} \supseteq \mathbb{D}_A$, i.e., the domain of the adjoint of an operator is *larger* than that of the operator itself. In that case the equality $(\chi\,,\, A\psi) = (A\chi\,,\, \psi)$ for all $\psi, \chi \in \mathbb{D}_A$ merely means that the operator A is **symmetric**.[2] Then, provided certain conditions are met, it is possible to find a so-called **self-adjoint extension** (or extensions) of the operator. Broadly speaking, this is done by enlarging the domain of A and shrinking that of $A^\dagger$ till they match. The physical importance of the property of self-adjointness arises from the fact that, in quantum mechanics, observables are represented by self-adjoint operators. Such operators have only real eigenvalues.

Projection operators: In general, given an orthonormal basis $\{|\phi_j\rangle\}$ in an LVS, the set of operators $\{|\phi_i\rangle\langle\phi_j|\}$ forms a basis for the operators acting on the vectors in the LVS. Of these, the 'diagonal' members of the set, namely, $P_j = |\phi_j\rangle\langle\phi_j|$, are projection operators. It is easy to see that

$$P_j^2 = P_j\,, \quad P_j\,(I - P_j) = 0\,, \quad \text{and} \quad P_j = P_j^\dagger\,.$$

These properties serve to *define* projection operators, in general.

The norm of an operator: Let A be a linear operator acting on the vectors in an LVS. The square of the **norm** $\|A\|$ of A is defined as the *least upper bound* or *supremum* of the ratio $(A\phi\,,\, A\phi)/(\phi\,,\, \phi)$ as $|\phi\rangle$ runs over all the vectors in the domain of A. That is,

$$\|A\|^2 = \sup_{|\phi\rangle\,\in\,\mathbb{D}_A} \frac{(A\,\phi\,,\, A\,\phi)}{(\phi\,,\, \phi)} = \sup_{|\phi\rangle\,\in\,\mathbb{D}_A} \frac{\langle\phi|A^\dagger\,A|\phi\rangle}{\langle\phi|\phi\rangle}\,.$$

Hence

$$\|A\| = \sup_{|\phi\rangle\,\in\,\mathbb{D}_A} \frac{\|A\,\phi\|}{\|\phi\|}\,.$$

[2] In the physics literature, we often say A is **hermitian**. Strictly speaking, however, the term 'hermitian' applies to operators that are symmetric as well as bounded.

If a is any scalar, then the norm of the operator $a\,A$ is given by

$$\|aA\| = |a|\,\|A\|.$$

The norm of a combination of operators satisfies the inequality

$$\|AB\| \leq \|A\|\,\|B\|.$$

Bounded and unbounded operators: An operator A is a **bounded operator** if $\|A\| < \infty$. If the norm of A is infinite, then A is an **unbounded operator**.

Several identities and relationships that one takes for granted based on their validity for finite-dimensional matrices are not necessarily valid for unbounded operators. Hence, as already mentioned, caution must be exercised when dealing with such operators, which occur quite frequently in quantum mechanics.

1. Let A and B be linear operators in an LVS, with respective domains $\mathbb{D}_A\,,\,\mathbb{D}_B$ and ranges $\Delta_A\,,\,\Delta_B$. What are the domains of the operators AB and BA?

2. Let $|\phi\rangle = (x_1\,, x_2\,, x_3\,, \ldots) \in \ell_2\,$. Consider operators $A_1\,, A_2\,, A_3\,, A_4\,, A_5$ whose actions on an element of the linear space are given, respectively, by

$$\begin{aligned}
A_1|\phi\rangle &= (x_2\,,\, x_3\,,\, x_4\,, \ldots), \\
A_2|\phi\rangle &= (0\,,\, x_1\,,\, x_2\,,\, x_3\,, \ldots), \\
A_3|\phi\rangle &= (1!\,x_1\,,\, 2!\,x_2\,,\, 3!\,x_3\,, \ldots), \\
A_4|\phi\rangle &= (x_1/1!\,,\, x_2/2!\,,\, x_3/3!\,, \ldots), \\
A_5|\phi\rangle &= (2x_1\,,\, x_2\,,\, x_3\,, \ldots)
\end{aligned}$$

Examine whether each of the operators $A_1\,, \ldots, A_5$ (i) has an inverse; and (ii) is bounded; if so, find the value of the norm of the operator concerned.

3. We have seen that the momentum operator of a particle moving on the x-axis has the representation $-i\hbar\,d/dx$ when acting on position-space wave functions $\psi(x,t)$. This is a direct consequence of the fundamental canonical commutation relation $[x,p] = i\hbar\,I$ between the position and momentum operators, where I is the unit operator. (We shall generally omit the superscript $\hat{}$ that is used sometimes to denote operators.) More generally, for three-dimensional motion, the momentum operator has the representation $-i\hbar\nabla$ when acting on position-space wave functions $\psi(\mathbf{r},t)$. This is the underlying reason why differential operators occur so frequently in quantum mechanics. We have also seen why the space $\mathcal{L}_2$ occurs naturally in quantum mechanics.

In the vector space $\mathcal{L}_2(-\infty\,,\,\infty)$ of square-integrable functions of a real variable x, find the adjoints of the following operators. Here a is a real constant, and m, n are positive integers.

(i) $x\,d/dx$ (ii) $x^2 + d^2/dx^2$ (iii) $\exp(i\,a\,x)$ (iv) $\exp(i\,a\,d/dx)$ (v) $x^m\,d^n/dx^n$.

4. Use the Cauchy-Schwarz inequality in an appropriate function space to show that

$$\int_{-\infty}^{\infty} dx\,\frac{e^{-x^2}}{(x^2+1)^{1/2}} < \pi^{3/4}\,.$$

5. Which of the following are bounded operators in $\mathcal{L}_2(-\infty\,,\,\infty)$?

$$\text{(i)}\, d/dx \quad \text{(ii)}\, x^n \;(n = 1,\, 2,\, \dots) \quad \text{(iii)}\, e^{-x^2/2} \quad \text{(iv)}\, (x^2+1)^{-1}.$$

6. The commutation relations

$$[x, I] = 0,\;\; [p, I] = 0,\;\; [x, p] = i\hbar I$$

between the position operator x, momentum operator p and the unit operator I specify a **Lie algebra**, called the **Heisenberg algebra**.[3]

(a) Show that all functions of x and p up to *quadratic* functions also form an algebra: that is, linear combinations of the operators I, x, p, x^2, p^2, xp and px form a closed algebra in the sense that their mutual commutators are again linear combinations of these operators.

(b) Verify that, once polynomials of any order *higher than quadratic* are considered, no such closed algebra is possible with *finite order* polynomials: polynomials of arbitrarily high order are generated by the commutators. The only possible algebra then involves *all* powers of the operators x and p. (This is called the W_∞ **algebra.)**

7. A linear operator a and its adjoint $a^\dagger$ in a certain LVS are found to satisfy the commutation rule $[a, a^\dagger] = I$, where I is the unit operator.[4]

(a) Find the commutators $[a^n\,,\, a^\dagger]$ and $[a\,,\, (a^\dagger)^n]$, where n is any positive integer.

(b) Hence find a simpler expression for the operator $e^a\, a^\dagger\, e^{-a}$.

8. An extension of the uncertainty principle: Let A and B be the self-adjoint operators corresponding to two of the observables of a system, and let

$$AB - BA = -i\,C \quad \text{and} \quad AB + BA = D.$$

Thus C and D are also self-adjoint operators. Consider the state given by

$$|\Psi\rangle = (A + i\alpha B)|\Phi\rangle,$$

where α is an arbitrary complex number and $|\Phi\rangle$ is an arbitrary state of the system. Using the fact that $\langle\Psi|\Psi\rangle \geq 0$ for all α, show that

$$(\Delta A)^2(\Delta B)^2 \geq \tfrac{1}{4}\big(\langle C\rangle^2 + \langle D\rangle^2\big).$$

[3] Recall that the concept of a Lie algebra has been introduced in the Classical Physics course. In that context, the Poisson bracket operation specifies the Lie algebra of functions of the phase space variables $(q_1\,, \dots, q_n\,,\, p_1\,, \dots, p_n)$ of a classical Hamiltonian system with n degrees of freedom.

[4] As you know, this commutation relation, together with the obvious ones $[a, I] = 0 = [a^\dagger, I]$, is just the Heisenberg algebra, written in terms of suitable dimensionless linear combinations of x and p.

Operator identities

Identities between mutually noncommuting operators are of great importance and use, as they are required very frequently in quantum mechanical calculations. What follows are some of the most common of these identities. Let A and B be linear operators in an LVS with a common domain. In general, A and B do *not* commute with each other, that is, $[A, B] \equiv AB - BA \neq 0$.

1. Perturbation expansion for the inverse of an operator: Frequently, we face the problem of finding the inverse of an operator of the form $(A + \epsilon\, B)$, where the inverse A^{-1} of A is known, and ϵ is a scalar of sufficiently small magnitude such that $\|\epsilon\, B\| \ll \|A\|$. We can then write a so-called **perturbation expansion** for the inverse $(A + \epsilon\, B)^{-1}$ (that is, an infinite series in powers of ϵ), as follows:

$$(A + \epsilon\, B)^{-1} = A^{-1} - \epsilon\, A^{-1}\, B\, A^{-1} + \epsilon^2\, A^{-1}\, B\, A^{-1}\, B\, A^{-1} + \ldots$$

Establish this result by starting with the identity

$$(A + \epsilon\, B)^{-1} = A^{-1} - \epsilon\, A^{-1}\, B\, (A + \epsilon\, B)^{-1}.$$

2. Hadamard's lemma is an extremely useful operator identity, from which a host of other operator identities can be derived. Let λ denote a scalar constant. Then

$$e^{\lambda\, A}\, B\, e^{-\lambda\, A} = B + \lambda\, [A, B] + \frac{\lambda^2}{2!}\, \big[A, [A, B]\big] + \frac{\lambda^3}{3!}\, \Big[A, \big[A, [A, B]\big]\Big] + \cdots .$$

Derive this result by defining the operator-valued function

$$F(\lambda) = e^{\lambda\, A}\, B\, e^{-\lambda\, A}.$$

Now obtain a first order differential equation (in λ) satisfied by $F(\lambda)$, and solve it, using the boundary condition $F(0) = B$.

Hadamard's lemma may be regarded as an identity between two analytic functions of the complex variable λ. The result is valid, by analytic continuation, for all complex λ satisfying $|\lambda| < \infty$. Re-labeling λ as $i\lambda$, we have a useful form of the lemma, namely,

$$e^{i\lambda\, A}\, B\, e^{-i\lambda\, A} = B + i\lambda\, [A, B] - \frac{\lambda^2}{2!}\, \big[A, [A, B]\big] - i\frac{\lambda^3}{3!}\, \Big[A, \big[A, [A, B]\big]\Big] + \cdots .$$

As I have already indicated, Hadamard's lemma is the starting point for the derivation of a large number of operator identities and relations.

3. Another useful operator relation that is closely related to Hadamard's lemma is as follows. Let A and B be two operators that do not commute with each other, in general. Define the operator B_t by

$$B_t = e^{iAt}\; B\; e^{-iAt},$$

where t is a parameter. (A and B do not depend on t.) Verify that B_t is a solution of the integral equation

$$B_t = B + i\, \Big[A\,,\, \int_0^t dt'\, B_{t'}\Big].$$

The Zassenhaus formula: It is often required to find the exponential of a linear combination of A and B. Since A and B do not commute with each other, this *cannot* be written as the exponential of A times the exponential of B. In general, $\exp(A+B)$ can only be expressed as an infinite product of operators of the form

$$e^{A+B} = e^A\ e^B\ e^{Z_1}\ e^{Z_2}\ e^{Z_3}\ \ldots$$

where

$$\left.\begin{array}{lcl} Z_1 & = & -\frac{1}{2}\,[A,B] \\ Z_2 & = & \frac{1}{6}\big[A\,,\,[A,B]\big] + \frac{1}{3}\big[B\,,\,[A,B]\big] \\ Z_3 & = & -\frac{1}{24}\Big[A\,,\,\big[A\,,\,[A,B]\big]\Big] - \frac{1}{8}\Big[A\,,\,\big[B\,,\,[A,B]\big]\Big] - \frac{1}{8}\Big[B\,,\,\big[B\,,\,[A,B]\big]\Big] \\ \ldots & \ldots & \ldots\ \ldots\ \ldots \end{array}\right\}$$

This is the Zassenhaus formula. The subsequent terms in the product involve higher-order multiple commutators that can be determined by a systematic but quite tedious iterative procedure.

The Baker-Campbell-Hausdorff (BCH) formula is the complement of the Zassenhaus formula, in the sense that it expresses the product of exponentials, $e^A\,e^B$, in terms of the exponential of an infinite sum of operators involving multiple commutators. Setting $[A,B]=C$, the formula is

$$(\exp\,A)\,(\exp\,B) = \exp\,\Big\{A+B+\tfrac{1}{2}C+\tfrac{1}{12}[A\,,\,C]-\tfrac{1}{12}[B\,,\,C]-\tfrac{1}{24}\big[B\,,\,[A\,,\,C]\big]+\cdots\Big\},$$

where $\cdots$ in the exponent on the right-hand side stands for an infinite sum of higher-order multiple commutators. As in the case of the Zassenhaus formula, the successive terms in the sum can be found by a recursive procedure.

4. In specific cases, if more information is available about the multiple commutators that appear in the Zassenhaus and BCH formulas, these formulas may be simplified somewhat. The simplest of these special cases, and the most important one, obtains when both A and B commute with their commutator $C=[A,B]$. (Sometimes this happens because C is just a constant multiple of the unit operator, but this is not necessary for the validity of the results that follow below.) The Zassenhaus and BCH formulas can then be derived in a fairly simple manner.

(a) Show that, if $[A,C]=0=[B,C]$, then

$$e^{A+B} = e^A\,e^B\,e^{-\frac{1}{2}[A,B]}\,.$$

You can derive this formula this by obtaining and solving a first-order differential equation for the operator $F(\lambda)$ defined as

$$F(\lambda) = e^{\lambda(A+B)},$$

where λ is a scalar (not an operator). Use the obvious boundary condition $F(0)=I$. Keep track of the fact that A and B do not commute with each other.

(b) Similarly show that, if $[A,C]=0=[B,C]$, then

$$e^A\,e^B = e^{A+B+\frac{1}{2}[A,B]}\,.$$

(c) Apply the result to the important case $A = iax\,,\ B = ibp$ where a and b are real scalars and x, p are the canonical position and momentum operators in one dimension, to find the commutator $[e^{iax}\,,\, e^{ibp}]$. This is called the **Weyl form** of the canonical commutation relation.

5. Here is a related but slightly different way of arriving at the Zassenhaus formula when the commutator of two operators is the unit operator. Let A and B be two operators such that $[A, B] = I$, the unit operator. Consider the linear combination $L = \alpha A + \beta B$, where α and β are arbitrary complex scalars (not operators).

(a) Show that $\dfrac{\partial L^n}{\partial \alpha} = nAL^{n-1} - \frac{1}{2}n(n-1)\beta L^{n-2}$.

(b) Show that $\dfrac{\partial\, e^L}{\partial \alpha} = \big(A - \frac{1}{2}\beta\big)\, e^L$.

(c) Integrate this last equation suitable to show that $e^{\,\alpha A + \beta B} = e^{\,\alpha A} e^{\,\beta B} e^{-\frac{1}{2}\alpha\beta}$.

Apply this to the important case $B = -a$, $A = a^\dagger$, so that $[A, B] = [a, a^\dagger] = 1$. Setting $\beta = \alpha^*$, we get the important relation

$$e^{\alpha\, a^\dagger - \alpha^*\, a} = e^{\alpha\, a^\dagger}\, e^{-\alpha^*\, a}\, e^{-\frac{1}{2}|\alpha|^2}\,.$$

The operator on the left-hand side is called the **displacement operator**. It generates **coherent states**, as we will see a little later.

Motion in one dimension

Many of the basic principles, properties and consequences of quantum mechanics can be illustrated very effectively in the case of a particle moving in one spatial dimension, the counterpart of a classical Hamiltonian system with one degree of freedom. I consider below some of the prototypical problems in this regard.

1. Wave packet dynamics of a free particle: Consider a particle moving freely in one dimension (the x-axis). As there is no force acting upon it, in the classical case it would have a definite momentum, say p_0 . The corresponding quantum mechanical momentum eigenstate is represented, in the position basis, by a wave function proportional to $e^{-ip_0x/\hbar}$ (i.e., a plane wave.) But such a wave function is not normalizable in $(-\infty, \infty)$. One way of getting around this problem is to confine the particle to a large but finite interval on the x-axis (a 'box'). Another way is to give up a strict momentum eigenstate, and to use a normalizable superposition of plane waves peaked (in wave number) about the wave number $p_0/\hbar$. Let's examine the time evolution of such a wave packet.

The most common superposition of this kind uses a **Gaussian wave packet** that is centered in momentum about p_0, and in position about some point x_0, to start with. Accordingly, we start with an initial state $|\Psi\,(0)\rangle$ of the particle at $t = 0$ that is represented by the position-space wave function

$$\langle x|\Psi\,(0)\rangle \equiv \psi(x,0) = \frac{1}{(\pi\sigma^2)^{1/4}}\, e^{-ip_0x/\hbar}\, e^{-(x-x_0)^2/2\sigma^2},$$

where σ is a positive constant. The positional probability density of the particle is a Gaussian centred about the point x_0 , with a width proportional to σ.

(a) Check that the wave function is normalized to unity, i.e., $\int_{-\infty}^{\infty} dx\, |\psi(x,0)|^2 = 1$.

The momentum-space wave function at any instant of time is the Fourier transform of the position-space wave function, and is given by

$$\widetilde{\psi}(p,t) \equiv \langle p|\Psi\,(t)\rangle = \int_{-\infty}^{\infty} dx\, \langle p|x\rangle\langle x|\Psi\,(t)\rangle = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} dx\, e^{-ipx/\hbar}\, \psi(x,t).$$

We have used the relation $\langle p|x\rangle = (2\pi\hbar)^{-1/2}\, e^{-ipx/\hbar}$. [5]

(b) Show that the normalized momentum-space wave function of the particle at $t = 0$ is given by

$$\widetilde{\psi}(p,0) = \Big(\frac{\sigma^2}{\pi\hbar^2}\Big)^{1/4} e^{ix_0(p-p_0)/\hbar}\, e^{-\sigma^2(p-p_0)^2/2\hbar^2}.$$

Apart from the phase factor $\exp\,[ix_0(p-p_0)/\hbar]$, this is again a Gaussian in p centred about the value p_0 . Note that the width of the Gaussian is now proportional to $1/\sigma^2$, i. e., it is proportional to the *reciprocal* of the width of the wave packet in position space. This is in accord with the general property that a narrow distribution in x implies a wide one in p, and vice versa.

[5] This is the usual normalization convention. It follows that $\langle x|p\rangle = \langle p|x\rangle^* = (2\pi\hbar)^{-1/2}\, e^{ipx/\hbar}$.

(c) Verify that the initial expectation values of the position and momentum are $\langle x(0)\rangle = x_0$ and $\langle p(0)\rangle = p_0$, respectively. Evaluate the initial uncertainties $\Delta x(0)$ and $\Delta p(0)$ at $t = 0$. Note that the uncertainty product $\Delta x(0)\,\Delta p(0) = \frac{1}{2}\hbar$. The initial state is therefore a **minimum uncertainty state**.

The time evolution of the state of the particle is given, of course, by the Schrödinger equation, $(i\hbar)\, d|\Psi(t)\rangle/dt = H|\Psi(t)\rangle$. The formal solution to this equation is $|\Psi(t)\rangle = \exp(-iHt/\hbar)\,|\Psi(0)\rangle$. The problem is then to evaluate the exponential of the Hamiltonian. Since $H = p^2/(2m)$ in the case of a free particle, and does not involve the position operator at all, it is obvious that the problem is most easily solved in the momentum basis. In this basis, the operator $\exp(-iHt/\hbar)$ is just multiplication by $\exp[-ip^2t/(2m\hbar)]$. This makes it trivial to write down the wave function $\widetilde{\psi}(p,t)$. We have

$$\begin{aligned}\widetilde{\psi}(p,t) &= \langle p\,|\Psi(t)\rangle = \langle p\,|\,e^{-iHt/\hbar}\,|\Psi(0)\rangle = \langle p\,|\,e^{-ip^2t/(2m\hbar)}\,|\Psi(0)\rangle \\ &= e^{-ip^2t/(2m\hbar)}\,\langle p|\Psi(0)\rangle = e^{-ip^2t/(2m\hbar)}\,\widetilde{\psi}(p,0).\end{aligned}$$

(d) Write down $\widetilde{\psi}(p,t)$ explicitly, and evaluate its inverse Fourier transform to determine the position-space wave function $\psi(x,t)$, according to

$$\psi(x,t) = \frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty} dp\, e^{ipx/\hbar}\,\widetilde{\psi}(p,t).$$

(e) Verify that this wave function remains normalized, i.e., $\int_{-\infty}^{\infty} dx\,|\psi(x,t)|^2 = 1$.

(f) Show that the expectation values of p and x at any time t are given by

$$\langle p(t)\rangle = p_0 = \langle p(0)\rangle, \quad \text{while} \quad \langle x(t)\rangle = x_0 + \frac{p_0\,t}{m} = \langle x(0)\rangle + \frac{p_0\,t}{m}\,.$$

In other words, the expectation values of the position and the momentum are related to each other in exactly the way in which the position and momentum of a classical free particle would be related. This is a special case of what is known as **Ehrenfest's Theorem**.

(g) Show that the uncertainty in the momentum at any time t, $\Delta p(t)$, remains equal to its value at $t = 0$. Evaluate $\Delta x(t)$ to show that the width of the wave packet in position space broadens as t increases.

Hence the uncertainty product $\Delta x(t)\,\Delta p(t)$ increases with time, and the state of the particle is no longer a minimum uncertainty state for any $t > 0$. The **dispersion** of the wave packet in position space is a consequence of the fact that the relation between (the eigenvalues of) the energy and the momentum is not a linear one for a free non-relativistic particle: if we set $E = \hbar\omega$ and $p = \hbar k$, the relation between the frequency and wave number for a free particle reads $\omega(k) = \hbar k^2/(2m)$. Hence the wave velocity ω/k is not identically equal to the group velocity $d\omega/dk$, and dispersion occurs.

2. Free particle in a box: The energy levels and the corresponding normalized position-space wave functions of a particle moving freely in a one-dimensional box $(0 < x < L)$ are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad \text{and} \quad \phi_n(x) = \begin{cases} \sqrt{2/L}\,\sin(n\pi x/L), & 0 < x < L \\ 0, & \text{all other } x \end{cases}$$

where $n = 1, 2, \ldots$. Although the wave function

$$\phi_n(x) = \sqrt{\frac{2}{L}} \left(\frac{e^{in\pi x/L} - e^{-in\pi x/L}}{2i} \right)$$

looks like a superposition of two plane waves (of wave numbers $n\pi/L$ and $-n\pi/L$, respectively), you must *not* jump to the conclusion that the particle is in a superposition of just two momentum eigenstates when it is in an eigenstate of the Hamiltonian. This erroneous conclusion appears to be supported by the fact that the particle is 'free' inside the box, and in the classical case it merely bounces back and forth between $x = 0$ and $x = L$, the *magnitude* of its momentum being conserved in time. In fact, however, there is a continuous distribution of momentum in an eigenstate of H, as you will see shortly.

(a) Verify that the set of wave functions $\{\phi_n(x)\}$ satisfies the orthonormality condition

$$\int_{-\infty}^{\infty} dx\, \phi_n(x)\, \phi_l(x) = \delta_{nl}$$

and the completeness relation

$$\sum_{n=1}^{\infty} \phi_n(x)\, \phi_n(x') = \delta(x - x').$$

(b) Find the corresponding set of momentum-space wave functions, given by

$$\widetilde{\phi}_n(p) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} dx\, e^{-ipx/\hbar}\, \phi_n(x).$$

It is important to note that $\widetilde{\phi}_n(p)$ is *not* an eigenfunction of the momentum operator. Although the system has been termed a 'free particle in a box', the fact is that the particle is in a potential that is not identically equal to zero for *all* x. Instead, we have

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{for all other } x. \end{cases}$$

Therefore p does not commute with the Hamiltonian of the particle, and a stationary state of the particle is not a momentum eigenstate as well. Nor is it a superposition of just *two* momentum eigenstates corresponding to momentum eigenvalues $\pm n\pi\hbar/L$, even though the form of the position-space eigenfunction $\phi_n(x)$ might suggest that this is so. The explicit expression for $\widetilde{\phi}_n(p)$ should make it amply clear that the momentum-space wave function is spread out over *all* values of p.

(c) Write down the momentum-space probability density $|\widetilde{\phi}_n(p)|^2$ when the particle is in the stationary state corresponding to energy E_n, and simplify the expression.

(d) Sketch the probability density of the momentum in the ground state,

$$|\widetilde{\phi}_1(p)|^2 = \frac{4\pi L\hbar^3}{(p^2L^2 - \pi^2\hbar^2)^2} \cos^2\left(\frac{pL}{2\hbar}\right), \qquad (-\infty < p < \infty)$$

as a function of p.

(e) Calculate the position and momentum uncertainties $(\Delta x)_n$ and $(\Delta p)_n$ in the energy eigenstate $\phi_n(x)$, and hence write down the value of the uncertainty product $(\Delta x)_n\,(\Delta p)_n$. Note that the uncertainty product is larger than its lowest allowed value $\frac{1}{2}\hbar$ even in the ground state of the particle.

3. Particle subjected to a constant force: A particle of mass m moves in one dimension under a uniform, constant force F. Its Hamiltonian is thus

$$H = \frac{p^2}{2m} - Fx.$$

(a) Let E denote an eigenvalue of H (i.e., an 'energy eigenvalue'). What are the allowed values of E? (This should be obvious on physical grounds.)

(b) Write down the time-independent Schrödinger equation for the *momentum-space* wave function $\widetilde{\phi}_E(p)$ corresponding to the eigenvalue E.

(c) Normalize the solution $\widetilde{\phi}_E(p)$ such that

$$\int_{-\infty}^{\infty} dp\, \widetilde{\phi}^*_E(p)\, \widetilde{\phi}_{E'}(p) = \delta(E - E').$$

4. Reflection and transmission in the presence of a potential barrier: Consider a quantum mechanical particle of mass m moving on the x-axis in the presence of a potential barrier given by

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0\,, & x > 0 \end{cases}$$

where V_0 is a positive constant.

(a) If the energy E of the particle is greater than V_0, show that the reflection and transmission coefficients are given by

$$R = \left(\frac{k - k'}{k + k'}\right)^2 \quad \text{and} \quad T = \frac{4kk'}{(k + k')^2}$$

respectively, where $\hbar k = \sqrt{2mE}$ and $\hbar k' = \sqrt{2m(E - V_0)}$.

(b) What happens to R as (i) $E \to V_0$ from above, and (ii) E becomes very much larger than V_0?

(c) What happens in the case $0 < E < V_0$?

5. Rectangular potential barrier: Now consider the potential barrier

$$V(x) = \begin{cases} V_0\,, & 0 \le x \le L \\ 0 & \text{otherwise} \end{cases}$$

where V_0 is a positive constant.

(a) For $E > V_0$, show that the transmission coefficient is given by

$$T = \frac{(2kk')^2}{(k^2 - k'^2)^2 \sin^2(k'L) + (2kk')^2}.$$

(b) Calculate the reflection coefficient R and verify that $R + T = 1$.

(c) Pass to the limit $L \to 0$ and $V_0 \to \infty$ such that $\lim (V_0\, L) = \lambda$. Verify that the transmission coefficient T is now given by

$$T = \frac{2E\hbar^2}{2E\hbar^2 + m\lambda^2}\,.$$

(d) Show that this last expression precisely the transmission coefficient in the case of the δ-function potential barrier $V(x) = \lambda\,\delta(x)$.

(e) For $0 < E < V_0$, show that the transmission coefficient becomes

$$T = \frac{(2k\kappa')^2}{(k^2 + \kappa'^2)^2\,\sinh^2(\kappa' L) + (2k\kappa')^2}\,,$$

where $\hbar\kappa' = \sqrt{2m(V_0 - E)}$.

The linear harmonic oscillator

Energy eigenvalues and eigenfunctions: Here is a quick recapitulation of the basic properties of the quantum mechanical linear harmonic oscillator. The importance of the harmonic oscillator is not restricted to the fact that it is a completely solvable quantum mechanical problem. It is closely related to systems with many degrees of freedom, such as collections of bosons, quantum fields (including radiation) satisfying Bose statistics, etc.

The Hamiltonian of the linear harmonic oscillator is given by

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 \, x^2,$$

where the position and momentum operators satisfy the commutation relation $[x\,,\,p] = i\hbar I$, I being the unit operator. It is very convenient to introduce the dimensionless position and momentum according to

$$\xi = x \left(\frac{m\omega}{\hbar}\right)^{1/2}, \quad \eta = \frac{1}{(m\omega\hbar)^{1/2}}\, p.$$

Then

$$H = \frac{1}{2}\hbar\omega\,(\xi^2 + \eta^2), \quad \text{where} \quad [\xi\,,\,\eta] = i\,I.$$

The operators $a^\dagger$ and a are defined as

$$a = \frac{1}{\sqrt{2}}\,(\xi + i\eta), \quad a^\dagger = \frac{1}{\sqrt{2}}\,(\xi - i\eta).$$

The fundamental commutation relation now becomes $[a\,,\,a^\dagger] = 1$,[6] while the Hamiltonian reads

$$H = \hbar\omega\left(a^\dagger\, a + \tfrac{1}{2}\right).$$

The eigenvalues of $a^\dagger\, a$ are nondegenerate, and are given by the set of nonnegative integers $0, 1, \ldots$. The combination $a^\dagger\, a$ is therefore called the **number operator**. It follows at once that the eigenvalues of H are also nondegenerate, and are given by

$$E_n = \hbar\omega\,\left(n + \tfrac{1}{2}\right), \quad \text{where} \quad n = 0, 1, \ldots\,.$$

The corresponding eigenstates $\{|\,n\,\rangle\}$, satisfying the eigenvalue equation $a^\dagger\, a\,|\,n\,\rangle = n\,|\,n\,\rangle$, are called **Fock states**. They form a complete orthonormal set. The ground state $|\,0\,\rangle$ is also called the **vacuum state**.[7] The action of a and $a^\dagger$ on $|\,n\,\rangle$ is given by

$$a\,|0\rangle = 0, \quad a\,|\,n\,\rangle = \sqrt{n}\,|n-1\rangle, \quad a^\dagger\,|\,n\,\rangle = \sqrt{(n+1)}\,|n+1\rangle.$$

This explains why a and $a^\dagger$ are termed the **raising** and **lowering operators**, respectively. It is most important to note that the eigenvalue spectra of $a^\dagger\, a$, and therefore H, are bounded from below, and that there exists a state $|\,0\,\rangle$ that yields zero when acted upon by a.

The normalized position-space wave function of the oscillator in the stationary state $|\,n\,\rangle$ is $\phi_n(x) \equiv \langle x|\,n\,\rangle$. It is the regular solution of the differential equation

$$-\frac{\hbar^2}{2m}\,\frac{d^2\phi_n}{dx^2} + \frac{1}{2} m\omega^2 x^2 \phi_n = E_n\,\phi_n\,,$$

[6] In a slight abuse of notation, we often write 1 for the unit operator. No confusion should arise as a result.

[7] In the context of the radiation field, this state corresponds to the zero-photon state.

and is given by

$$\phi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/(2\hbar)}\, H_n\big(x\sqrt{m\omega/\hbar}\big),$$

where H_n denotes the Hermite polynomial of order n. The first few of these polynomials are

$$H_0(u) = 1,\ H_1(u) = 2u,\ H_2(u) = 4u^2{-}2,\ H_3(u) = 8u^3{-}12u,\ H_4(u) = 16u^4{-}48u^2{+}12.$$

The Rodrigues formula for these polynomials is

$$H_n(u) = (-1)^n\, e^{u^2}\, \frac{d^n}{du^n}\, e^{-u^2}.$$

The generating function of the Hermite polynomials is given by

$$e^{-t^2+2tu} = \sum_{n=0}^{\infty} H_n(u) \frac{t^n}{n!}\,.$$

$H_n(u)$ is the regular solution of Hermite's differential equation,

$$\frac{d^2 H_n}{du^2} - 2u\, \frac{dH_n}{du} + 2n\, H_n = 0.$$

The oscillator eigenfunctions $\phi_n(x)$ form a complete orthonormal set of functions in $\mathcal{L}_2(-\infty\,,\,\infty)$. The orthonormality relation is

$$\int_{-\infty}^{\infty} dx\, \phi_n(x)\, \phi_l(x) = \delta_{nl}\,,$$

while the completeness relation is

$$\sum_{n=0}^{\infty} \phi_n(x)\, \phi_n(x') = \delta(x - x').$$

1. Consider a linear harmonic oscillator in its ground state. Calculate the total probability that the position of the oscillator is (i) in the range $-(\hbar/2m\omega)^{1/2} \le x \le (\hbar/2m\omega)^{1/2}$; (ii) outside this range. Note that the regions in (i) and (ii), respectively, are the allowed and forbidden regions for a *classical* simple harmonic oscillator whose total energy is E_0.

2. Using operator methods, show that the expectation values of the kinetic energy and the potential energy of the oscillator in the stationary state $|\, n\,\rangle$ are equal. Hence show that their expectation values in an *arbitrary* normalizable state are equal.

3. A shifted harmonic oscillator: (This is a trivial problem!) Suppose a term is added to the Hamiltonian of thje linear harmonic oscillator, so that it is now given by

$$H = \hbar\omega\, \big(a^\dagger a + \tfrac{1}{2}\big) + \lambda(a + a^\dagger)\,,$$

where λ is a real constant.

(a) What does this new Hamiltonian correspond to, physically?

(b) Find the eigenvalues of this Hamiltonian.

(c) What value(s) should λ take in order that the ground state energy be exactly zero?

4. Other perturbations of the linear harmonic oscillator: Consider the perturbed Hamiltonian $H = H_0 + \lambda H'$, where

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

is the Hamiltonian of a linear harmonic oscillator, λ is a positive constant of appropriate physical dimensions, and H' is given, respectively, by (i) x^2 (ii) x^3 (iii) x^4. Calculate, in each case, the new energy levels correct to second order in the small parameter λ, and the corresponding eigenstates correct to first order in λ. Compare these with the exact expressions for these quantities in those cases, if any, in which the problem can be solved analytically.

5. Propagator for the linear harmonic oscillator: In the foregoing, we have focused our attention on the stationary states of the linear harmonic oscillator. Here is an aspect of interest pertaining to the time-dependent problem. The time-dependent Schrödinger equation for a linear harmonic oscillator in the position basis is given by

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\psi(x,t)\ .$$

Verify that the solution to this equation is given by

$$\psi(x,t) = \int_{-\infty}^{\infty} dx'\ K(x,x';t)\ \psi(x',0),$$

where

$$K(x,x'\,;\,t) = \Big(\frac{m\omega}{2\pi i\hbar\sin\omega t}\Big)^{1/2}\ \exp\Big[\frac{im\omega}{2\hbar\sin\omega t}\big\{(x^2+x'^2)\cos\omega t - 2xx'\big\}\Big].$$

First check that $\psi(x,t)$ obeys the time-dependent Schrödinger equation. Next, check to see whether the proper initial condition is satisfied at $t = 0$, i. e., that $\psi(x,t)$ reduces to the given initial function $\psi(x,0)$.

The quantity $K(x,x'\,;\,t)$ is called the **propagator** because it takes us from the solution at time $t = 0$ to the solution at any subsequent instant of time $t > 0$. Note that $\psi(x,t)$ at any given point x depends on the initial wave function $\psi(x',0)$ at *all* points x'.

6. A pair of coupled harmonic oscillators: Before going on to other aspects of the linear harmonic oscillator, let us consider a pair of coupled harmonic oscillators. The coupling is such that the total Hamiltonian can be diagonalized and the energy levels computed exactly. This enables us to compare the results of perturbation theory with the corresponding exact expressions, thereby gaining some insight into the former.

The two-dimensional isotropic oscillator is given by the Hamiltonian

$$H_0 = \frac{p_1^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2 x_2^2\,,$$

where

$$[x_i\,,\,x_j] = 0,\ [p_i\,,\,p_j] = 0,\ [x_i\,,\,p_j] = i\hbar\,\delta_{ij}\,,$$

and the indices run over the values 1 and 2. Now consider the perturbed Hamiltonian $H = H_0 + \lambda H'$, where λ is a real constant and

$$H' = x_1\, x_2\,.$$

(a) The ground state energy of the unperturbed Hamiltonian is of course given by $E_0^{(0)} = (\frac{1}{2} + \frac{1}{2})\,\hbar\omega = \hbar\omega$. Show that, up to the second order in the coupling constant λ, the ground state energy of the perturbed oscillator is given by

$$E_0 = \hbar\omega + \frac{\lambda^2\hbar}{8m^2\omega^3}\,.$$

(b) The first excited state of the unperturbed Hamiltonian is doubly degenerate. It corresponds to the energy eigenvalue $E_1^{(0)} = 2\hbar\omega$. The corresponding normalized eigenstates may be taken to be the linear combinations

$$\frac{|\,1,0\,\rangle + |\,0,1\,\rangle}{\sqrt{2}} \quad \text{and} \quad \frac{|\,1,0\,\rangle - |\,0,1\,\rangle}{\sqrt{2}}$$

where $|n_1\,,\,n_2\,\rangle$ is an eigenstate of H_0 with energy $\hbar\omega(n_1 + n_2 + 1)$. Show that the perturbation lifts the degeneracy of the first excited state of the Hamiltonian, and that the energy level $E_1^{(0)} = 2\hbar\omega$ is split, to first order in λ, into the two energy levels

$$2\hbar\omega - \frac{\lambda\hbar}{2m\omega} \quad \text{and} \quad 2\hbar\omega + \frac{\lambda\hbar}{2m\omega}\,.$$

(c) It should be clear that the corresponding classical problem can be solved easily by changing variables. This remains true in the quantum mechanical case as well. Define

$$X = \frac{x_1 + x_2}{\sqrt{2}} \quad \text{and} \quad x = \frac{x_1 - x_2}{\sqrt{2}}\,,$$

and similarly

$$P = \frac{p_1 + p_2}{\sqrt{2}} \quad \text{and} \quad p = \frac{p_1 - p_2}{\sqrt{2}}\,.$$

Check out the commutation relations satisfied by these new operators. Write down the Hamiltonian H in terms of these operators, using the fact that

$$x_1\, x_2 = \frac{1}{2}(X^2 - x^2).$$

(d) Hence show that the exact energy levels (eigenvalues) of H are given by

$$E(n_1\,,\,n_2) = \hbar\omega_-\left(n_1 + \tfrac{1}{2}\right) + \hbar\omega_+\left(n_2 + \tfrac{1}{2}\right),$$

where n_1 and n_2 run over the values $0, 1, \ldots$ as usual, and

$$\omega_- = \sqrt{\omega^2 - \frac{\lambda}{m}}\,, \quad \omega_+ = \sqrt{\omega^2 + \frac{\lambda}{m}}\,.$$

Note that we must have $|\lambda| < m\omega^2$ in this problem. If $|\lambda| > m\omega^2$, the spectrum of the Hamiltonian is not bounded from below. (Examine what happens to the corresponding classical potential energy.)

Momentum-space wave functions of the oscillator: We return to the time-independent Schrödinger equation for the linear harmonic oscillator, and the associated eigenstates and eigenfunctions.

We know that the Fourier transform of a Gaussian function is again a Gaussian. This relationship is a special case of a more general fact, which is connected to yet another interesting aspect of the quantum mechanical harmonic oscillator. From this point onward, we set $\hbar, m$ and ω equal to unity, for convenience and notational simplicity.[8] The Hamiltonian is then $H = \frac{1}{2}(p^2+x^2)$, with eigenvalues $E_n = (n+\frac{1}{2})$. The position-space eigenfunctions $\phi_n(x)$ satisfy the Schrödinger equation

$$\Big(\frac{d^2}{dx^2} - x^2 + 2E_n\Big)\phi_n(x) = 0.$$

The normalized solutions are the $\mathcal{L}_2(-\infty\,,\,\infty)$ functions

$$\phi_n(x) == \frac{1}{\pi^{1/4}}\,\frac{1}{\sqrt{2^n\,n!}} e^{-x^2/2}\,H_n(x),$$

where $H_n(x)$ is the Hermite polynomial of order n.

Now consider the *momentum-space* eigenfunctions of H. These are given by $\widetilde{\phi}_n(p)$, which are also $\mathcal{L}_2(-\infty\,,\,\infty)$ functions satisfying the Schrödinger equation

$$\Big(\frac{d^2}{dp^2} - p^2 + 2E_n\Big)\widetilde{\phi}_n(p) = 0.$$

But this precisely the *same* equation as the one satisfied by the position-space eigenfunctions $\phi_n(x)$! This symmetry arises because the oscillator Hamiltonian is completely symmetrical in x^2 and p^2. As a consequence, the differential operator that acts on $\phi_n(x)$ to yield zero is exactly the same as the one that acts on $\widetilde{\phi}_n(p)$ to yield zero. The normalized momentum-space eigenfunctions must therefore be given by

$$\widetilde{\phi}_n(p) = \frac{\mu_n}{\pi^{1/4}}\,\frac{1}{\sqrt{2^n\,n!}} e^{-p^2/2}\,H_n(p),$$

where the constant μ_n must have unit modulus, i.e., $|\mu_n| = 1$. In other words, the position-space and momentum-space wave functions of the stationary states of the harmonic oscillator are exactly the same in functional form.

Eigenfunctions of the Fourier transform operator: The fact just stated leads to an interesting connection between the eigenfunctions $\{\phi_n\}$ and the Fourier transform operator.

We know that, in general, position-space and momentum-space wave functions corresponding to the same state are just Fourier transforms of each other: that is,

$$\widetilde{\psi}(p) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\; e^{-ipx}\,\psi(x),$$

with the inverse transformation

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dp\; e^{ipx}\,\widetilde{\psi}(p).$$

[8] These factors are easily restored in any of the expressions that follow, based on dimensional considerations.

(Recall that we have set $\hbar = 1$.) What we now see is that, for the oscillator eigenfunctions, the functional forms of ϕ_n and $\widetilde{\phi}_n$ are exactly the same. In other words, the functions

$$\frac{1}{\pi^{1/4}}\,\frac{1}{\sqrt{2^n\,n!}}e^{-x^2/2}\,H_n(x), \quad n = 0, 1, 2, \ldots$$

are, up to a possible multiplicative constant of unit modulus, normalized eigenfunctions of the Fourier transform *operator* in $\mathcal{L}_2(-\infty\,,\,\infty)$.

Let us elaborate on this a little further. The Fourier transform operator, which we may denote by $\mathcal{F}$, is an **integral operator** that acts on functions of a real variable to produce other functions. If we restrict our attention to functions in $\mathcal{L}_2(-\infty\,,\,\infty)$, then

$$\psi(x) \in \mathcal{L}_2(-\infty\,,\,\infty) \Longrightarrow (\mathcal{F}\psi)(x) \in \mathcal{L}_2(-\infty\,,\,\infty)$$

as well. That is, $\mathcal{F}$ takes functions belonging to $\mathcal{L}_2(-\infty\,,\,\infty)$ to other functions in the same function space. The **kernel** of the integral operator $\mathcal{F}$ is given by $F(p,x) = (2\pi)^{-1/2}e^{-ipx}$. That is,

$$(\mathcal{F}\psi)(p) \equiv \widetilde{\psi}(p) = \int_{-\infty}^{\infty} F(p,x)\,\psi(x)\,dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ipx}\,\psi(x)\,dx.$$

What we have found above is that, for the oscillator eigenfunctions ϕ_n, the function and its Fourier transform $\mathcal{F}\phi_n\,(\equiv \widetilde{\phi}_n)$ are the same in functional form. This means that these eigenfunctions are also eigenfunctions of the Fourier transform operator $\mathcal{F}$ itself. ϕ_n and $\widetilde{\phi}_n$ must therefore differ, if at all, only by an overall multiplicative constant, say μ_n. But ϕ_n and $\widetilde{\phi}_n$ must have the same norm, by **Parseval's Theorem**:

$$\int_{-\infty}^{\infty} |\phi_n(x)|^2\,dx = \int_{-\infty}^{\infty} |\widetilde{\phi}_n(p)|^2\,dp.$$

Therefore, since ϕ_n is normalized to unity, so is $\widetilde{\phi}_n$. Hence the multiplicative constant μ_n can only be a phase factor, i.e., a complex number of unit modulus. And this number μ_n must be an eigenvalue of the Fourier transform operator $\mathcal{F}$ when it acts on elements of the space $\mathcal{L}_2(-\infty\,,\,\infty)$.[9]

7. The next task is to determine the possible values of μ_n.

(a) Work out explicitly the Fourier transforms of the eigenfunctions $\phi_n(x)$ for $n = 0, 1, 2, 3$ and 4. You will need to use the expressions given for the first few Hermite polynomials given in the foregoing. You will also need the Gaussian integral

$$\int_0^{\infty} e^{-ax^2}\,x^r\,dx = \Gamma\left(\tfrac{1}{2}(r+1)\right)\Big/ 2a^{(r+1)/2}, \;\; (a > 0 \text{ and } r > -1)$$

where Γ is the gamma function.

(b) Verify that the eigenvalues of $\mathcal{F}$ in these cases are, respectively, 1, $-i$, -1, i and again 1. That is, check out that

$$\widetilde{\phi}_0(p) = \phi_0(p),\;\; \widetilde{\phi}_1(p) = -i\,\phi_1(p),\;\; \widetilde{\phi}_2(p) = -\,\phi_2(p),\;\; \widetilde{\phi}_3(p) = i\,\phi_3(p),$$

while $\widetilde{\phi}_4(p) = \phi_4(p)$ once again.

[9] Another argument to support the assertion that the eigenvalues of the Fourier transform operator must be complex numbers of unit modulus: $\mathcal{F}$ is a *unitary* operator.

We may therefore conjecture that the possible distinct eigenvalues of $\mathcal{F}$ are $+1$, $-i$, -1, and i. This is indeed the case.

(c) Check out directly that the square of the Fourier transform operator is just the **parity operator** $\mathcal{P}$, i.e., that

$$(\mathcal{F}^2\,\psi)(x) = (\mathcal{P}\psi)(x) = \psi(-x).$$

Since $\mathcal{P}^2 = I$, the fourth power of the Fourier transform operator is just the unit operator!

$$(\mathcal{F}^4\psi)(x) = \psi(x),\ \text{i. e., } \mathcal{F}^4 = I,\ \text{ the unit operator in } \mathcal{L}_2(-\infty\,,\,\infty).$$

It is then reasonable to expect that the eigenvalues of the operator $\mathcal{F}$ are just the fourth roots of unity. We conclude that:

- The oscillator eigenfunction $\phi_n(x)$ is also an eigenfunction of the Fourier transform operator $\mathcal{F}$ in $\mathcal{L}_2(-\infty\,,\,\infty)$, with eigenvalue $e^{-i\pi r/2}$, where $r = n \bmod 4$, so that $r = 0, 1, 2, 3$.

The eigenfunctions $\phi_n(x)$ are of course eigenfunctions of $\mathcal{P}$ as well, since $[H, \mathcal{P}] = 0$. This property is shared by all the bound state eigenfunctions of a symmetric potential ($V(x) = V(-x)$). What we now find is that $[H, \mathcal{F}] = 0$ for the special case of the *oscillator* Hamiltonian. The parity operator may be regarded as a 'square root' of the unit operator. The Fourier transform operator may be regarded as a 'square root' of the parity operator.

Representations of H, $\mathcal{P}$ and $\mathcal{F}$: In the position basis, the oscillator Hamiltonian is represented by the differential operator $H = \frac{1}{2}\big(x^2 - d^2/dx^2\big)$. The parity and Fourier transform operators have the respective actions

$$\psi(x) \xrightarrow{\mathcal{P}} \psi(-x) \quad \psi(x) \xrightarrow{\mathcal{F}} \widetilde{\psi}(x), \quad \psi(x) \in \mathcal{L}_2(-\infty\,,\,\infty).$$

$\mathcal{F}$ is represented by an integral operator in this basis. On the other hand, the Hamiltonian is represented in the Fock basis (i.e., in the basis of its own eigenstates) by the diagonal matrix $H = \mathrm{diag}\,(E_0\,,\,E_1\,,\,\dots)$, where $E_n = (n + \frac{1}{2})$. What about the parity and Fourier transform operators $\mathcal{P}$ and $\mathcal{F}$? As these operators commute with H, they too are representable by diagonal matrices, with their eigenvalues on the diagonal. In terms of projection operators, this means that we may write

$$H = \sum_{n=0}^{\infty} E_n\,|\,n\,\rangle\langle\,n\,|, \quad \mathcal{P} = \sum_{n=0}^{\infty}(-1)^n\,|\,n\,\rangle\langle\,n\,|, \quad \mathcal{F} = \sum_{n=0}^{\infty}(-i)^n\,|\,n\,\rangle\langle\,n\,|.$$

Coherent states of the harmonic oscillator

It turns out to be possible to find normalizable eigenstates of the lowering operator a, essentially because the spectrum of the number operator $a^\dagger a$ is bounded from below. (That is, there exists a state $|\,0\,\rangle$ that is 'annihilated' by a, i.e., a state such that $a\,|\,0\,\rangle = 0$.) These state are called **coherent states**,[10] and they have an enormous number of very interesting and important properties. These states and their various generalisations play a pivotal role in all of quantum optics, among other areas.[11]

1. Let $|\alpha\rangle$ denote an eigenstate of a with eigenvalue α, i.e., $a\,|\alpha\rangle = \alpha\,|\alpha\rangle$. The possible values of α will be determined shortly.

(a) Expand $|\alpha\rangle$ in the Fock basis, i.e., let $|\alpha\rangle = \sum_{n=0}^{\infty} c_n\,|\,n\,\rangle$. Substitute this in the eigenvalue equation for $|\alpha\rangle$, and determine the coefficients c_n recursively, by equating the coefficients of each individual Fock state on either side of the equation. Impose the normalization condition $\langle\,\alpha\,|\alpha\rangle = 1$, to arrive at the following expression for $|\alpha\rangle$ (after choosing the overall phase factor to be unity):

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\,|\,n\,\rangle.$$

Note that no condition whatsoever has been placed upon the eigenvalue α. Since we are able to find a normalizable eigenstate $|\alpha\rangle$ for *any arbitrary complex value* of the eigenvalue α, we must conclude that the eigenvalue spectrum of the lowering operator a is, in fact, the whole of the finite part of the complex plane. Recall that a is non-self-adjoint. Its eigenvalues can therefore be complex numbers, in general. We now find that its eigenvalue spectrum is actually doubly continuous (both $\alpha_1 \equiv \mathrm{Re}\,\alpha$ and $\alpha_2 \equiv \mathrm{Im}\,\alpha$ can take on values in $(-\infty, \infty)$.)

(b) Show that a similar argument does not work for the *raising* operator $a^\dagger$: that is, there can be no *normalizable* eigenstate of $a^\dagger$, in stark contrast to the case of a. Note the reason why: there is no state $|\,n\,\rangle$ such that $a^\dagger\,|\,n\,\rangle = 0$, i.e., there is no *upper* bound to the eigenvalue spectrum of $a^\dagger\,a$.

You can verify the foregoing statements in an alternative (but equivalent) way, by working in the position representation. Let $\psi_\alpha(x) \equiv \langle\,x\,|\alpha\rangle$ be the position-basis wave function corresponding to the CS $|\alpha\rangle$. The eigenvalue equation then gives $\langle\,x\,|\,a\,|\alpha\rangle = \alpha\,\langle\,x\,|\alpha\rangle = \alpha\,\psi_\alpha(x)$. Put $a = (x + ip)/\sqrt{2}$, and remember that p is represented by $-id/dx$ in the position basis. This leads to a first-order differential equation for $\psi_\alpha(x)$,

$$\frac{d\psi_\alpha}{dx} + (x - \sqrt{2}\,\alpha)\,\psi_\alpha = 0.$$

The solution is a shifted Gaussian in x, apart from a phase factor. It is clearly normalizable. In contrast, if $\chi_\beta(x)$ is the wave function corresponding to an eigenvalue β of the operator $a^\dagger$, the differential equation satisfied by it is

$$\frac{d\chi_\beta}{dx} - (x - \sqrt{2}\,\beta)\,\chi_\beta = 0.$$

The solution is obviously not normalizable in $(-\infty, \infty)$.

[10] I will use the abbreviation CS for 'coherent state'.

[11] In particular, the state of the radiation field in an ideal single mode laser is a CS. We will not be concerned here with this aspect of coherent states.

(c) Show that the normalized position-space wave function corresponding to the CS $|\alpha\rangle$ is given by

$$\psi_\alpha(x) = \pi^{-1/4}\, e^{-\frac{1}{2}(x-\sqrt{2}\,\alpha_1)^2}\; e^{i\alpha_2\,(\alpha_1-\sqrt{2}\,x)}.$$

(d) Hence show that the momentum-space wave function corresponding to the CS $|\alpha\rangle$ is given by

$$\widetilde{\psi}_\alpha(p) = \pi^{-1/4}\, e^{-(p-\sqrt{2}\,\alpha_2)^2/2}\; e^{i\alpha_1\,(\sqrt{2}\,p-\alpha_2)}.$$

The displacement operator: Using the fact that $(a^\dagger)^n\,|\,0\,\rangle = \sqrt{n!}\,|\,n\,\rangle$, $|\alpha\rangle$ can be re-expressed as

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\, e^{\alpha\, a^\dagger}\,|\,0\,\rangle.$$

Now, since $a\,|\,0\,\rangle = 0$, we have $a^n\,|\,0\,\rangle = 0$ for all positive integer values of n. Hence $e^{-\alpha^*\,a}\,|\,0\,\rangle = |\,0\,\rangle$. Therefore $|\alpha\rangle$ may be further re-written as

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\, e^{\alpha\, a^\dagger}\, e^{-\alpha^*\,a}\,|\,0\,\rangle.$$

Using the BCH formula, we find

$$e^{-\frac{1}{2}|\alpha|^2}\, e^{\alpha\, a^\dagger}\, e^{-\alpha^*\,a} = e^{\alpha\, a^\dagger - \alpha^*\,a} \stackrel{\text{def.}}{=} D(\alpha).$$

The operator $D(\alpha)$ is called the **displacement operator**, for a reason which will become clear shortly.[12] In terms of this operator, the CS $|\alpha\rangle$ is simply

$$|\alpha\rangle = D(\alpha)\,|\,0\,\rangle.$$

But the adjoint of D is $D^\dagger = e^{-(\alpha\, a^\dagger - \alpha^*\,a)}$. Since the operator $\alpha\, a^\dagger - \alpha^*\, a$ commutes with itself, it follows at once that $D\,D^\dagger = D^\dagger\,D = I$, i.e., that $D(\alpha)$ is a **unitary operator**. The CS $|\alpha\rangle$ is therefore nothing but a **unitarily transformed** vacuum state.[13]

This helps us understand why the position-space wave function $\psi_\alpha(x)$ and the momentum-space wave function $\widetilde{\psi}_\alpha(p)$ of a CS are also Gaussians, apart from a phase factor in each case. The significance of the parameters α_1 and α_2 also becomes clear: the peak of the Gaussian is *displaced* from 0 in the vacuum state to $\sqrt{2}\,\alpha_1$ in position space, and to $\sqrt{2}\,\alpha_2$ in momentum space.

2. Coherent states are minimum uncertainty states: Since $|\alpha\rangle$ is a unitarily transformed vacuum state, you might expect certain properties of $|\,0\,\rangle$ to be carried over to all coherent states.

(a) In the CS $|\alpha\rangle$, compute the expectation values of

$$x = \frac{a + a^\dagger}{\sqrt{2}},\quad p = \frac{a - a^\dagger}{i\sqrt{2}},\; x^2 \;\text{ and }\; p^2.$$

[12] We should write $D(\alpha, \alpha^*)$ because the operator D is parametrized by α as well as α^* (or the two independent variables α_1 and α_2). But it is customary to write just $D(\alpha)$, in a slight abuse of notation.

[13] The vacuum state itself is also a coherent state, of course, corresponding to $\alpha = 0$.

(b) Hence show that (in the units we have chosen) $\Delta x = \Delta p = 1/\sqrt{2}$ in this state, independent of α. Therefore the uncertainty product is $(\Delta x)(\Delta p) = \frac{1}{2}$ in any CS, i.e., all of them are minimum uncertainty states.

3. Non-orthogonality of CS: The states $\{|\alpha\rangle, \ \alpha \in \mathbb{C}\}$ are normalized to unity, but they are not mutually orthogonal.

(a) Show that, if α and β are any two distinct complex numbers, then

$$\langle \alpha | \, \beta \, \rangle = e^{-\frac{1}{2}(|\alpha|^2 + |\beta|^2) + \alpha^* \beta}$$

(b) Hence show that

$$|\langle \alpha | \, \beta \, \rangle|^2 = e^{-|\alpha - \beta|^2}.$$

The 'overlap' $|\langle \alpha | \, \beta \, \rangle|^2$ therefore decreases quite rapidly as the 'distance' $|\alpha - \beta|$ between the two states increases, but it is not identically equal to zero.

Over-completeness of CS: It can be shown that

$$\int d^2\alpha \, |\alpha\rangle\langle\alpha| = \pi \, I,$$

where I is the unit operator and $\int d^2\alpha$ stands for an integral over the whole of the complex plane, i. e., a double integral over all values of α_1 and α_2 in the ranges $\alpha_1 \in (-\infty, \infty)$ and $\alpha_2 \in (-\infty, \infty)$. The fact that the right-hand side has a factor $\pi \, (> 1)$ implies that the set of CS is an **over-complete set** of states.

It is of interest to ask whether there exist *subsets* of the set of CS that are complete sets. The determination of such sets is a nontrivial task. It is known, for instance, that the set of states for which α lies on the unit circle in the complex plane form a complete set; so does the set of states for which $\alpha = m + ni$, where m and n are integers; and so on.

4. The mean and variance of $a^\dagger \, a$ in a CS: The expectation value of the number operator $a^\dagger \, a$ in the Fock state $| \, n \, \rangle$ is of course $\langle \, n \, | \, a^\dagger \, a \, | \, n \, \rangle = n$, and hence $\langle \, 0 \, | \, a^\dagger \, a \, | \, 0 \, \rangle = 0$. In the case of the CS $|\alpha\rangle$, we have $a \, |\alpha\rangle = \alpha \, |\alpha\rangle$ and hence $\langle \alpha | \, a^\dagger = \alpha^* \, \langle \alpha |$. It follows immediately that the expectation value of the number operator in the CS $|\alpha\rangle$ is

$$\langle \alpha | \, a^\dagger \, a \, | \alpha \rangle = |\alpha|^2.$$

Show that the variance of the number operator $a^\dagger \, a$ in the CS $|\alpha\rangle$ is also equal to $|\alpha|^2$. Hence the standard deviation of this quantity, i.e., the uncertainty in $a^\dagger \, a$, is equal to $|\alpha|$ in the state $|\alpha\rangle$.

It turns out that *all* the higher cumulants of the number operator are also equal to $|\alpha|^2$ in the CS $|\alpha\rangle$. In the context of radiation, this is a consequence of the fact that the photon number in ideal, single-mode laser light has a Poisson distribution.

5. Use Hadamard's lemma to show that

$$D(\alpha) \, a \, D^\dagger(\alpha) = a - \alpha \quad \text{and} \quad D(\alpha) \, a^\dagger \, D^\dagger(\alpha) = a^\dagger - \alpha^*.$$

Again, these relations tell us why $D(\alpha)$ is termed the displacement operator. Under a unitary transformation by $D(\alpha)$,

$$\text{the state } \ | \, 0 \, \rangle \xrightarrow{D(\alpha)} |\alpha\rangle, \ \text{ while the operator } \ a \xrightarrow{D(\alpha)} D(\alpha) \, a \, D^\dagger(\alpha).$$

Hence the relation $a\,|\,0\,\rangle = 0$ is transformed to

$$D(\alpha)\,a\,|\,0\,\rangle = 0, \;\; \text{or} \;\; D(\alpha)\,a\,D^\dagger(\alpha)D(\alpha)\,|\,0\,\rangle = (a-\alpha)\,|\alpha\rangle = 0.$$

Viewed thus, the defining eigenvalue equation for a CS is nothing but a unitarily transformed or displaced version of $a\,|\,0\,\rangle = 0$.

$D(\alpha)$ **as an element of a Lie group**: We have mentioned already that the operators a, $a^\dagger$ and I are the generators of a Lie algebra, the Heisenberg algebra. Exponentiating a linear combination of these generators will then yield the general element of the corresponding **Lie group**. It is in this sense that $D(\alpha)$ is an element of the Heisenberg group.[14] The question of interest, then, is the group multiplication law.

6. Let α and β be any two complex numbers. Show that the displacement operator satisfies the following group composition rule:

$$D(\alpha)\,D(\beta) = D(\alpha+\beta)\,e^{\frac{1}{2}(\alpha\,\beta^* - \alpha^*\,\beta)} = D(\alpha+\beta)\,e^{i\,\mathrm{Im}\,(\alpha\,\beta^*)}\,.$$

Generalizations: Various generalizations of coherent states are possible. This topic has been studied in some detail, especially in the context of quantum optics. We have the **generalized coherent state** $|\,n,\alpha\rangle$ obtained by applying the displacement operator $D(\alpha)$ to the Fock state $|\,n\,\rangle$ (rather than the vacuum state $|\,0\,\rangle$) and normalizing the result; the **photon-added coherent state** $|\,\alpha,n\,\rangle$ obtained by operating on $|\alpha\rangle$ with $a^{\dagger\,n}$ and normalizing the result; and so on. Other transformations of the vacuum state are also of relevance. For instance,

[14] It involves two real parameters α_1 and α_2, in accord with the two nontrivial generators a and $a^\dagger$ of the Lie algebra.

QUIZ

1. Are the statements in quotation marks true or false?

(a) The position and momentum operators of a particle moving in one dimension satisfy the commutation relation $[x\,,\,p] = i\hbar\, I$, where I is the unit operator.

"It is possible to represent the operators x and p by hermitian $(n \times n)$ matrices where n is any positive integer."

(b) A particle moves in one dimension in the potential $V(x)$. The energy spectrum of the particle is discrete. The potential is symmetric about the origin, i. e., $V(-x) = V(x)$.

"It follows that the position-space wave function corresponding to any stationary state of the particle is an even function of x."

(c) A particle moves in space under the influence of a potential $V(\mathbf{r})$.

"The particle can never be in a state in which its kinetic energy and potential energy can simultaneously have precise values."

(d) Let A be the operator corresponding to a physical observable of a system with Hamiltonian H, and let $[A\,,\,H] \neq 0$. Then:

"No eigenstate of A can be a stationary state of the system."

(e) Let $A\,,\,B$ and C be operators corresponding to physical observables of a system, such that $[A\,,\,B] = 0$ and $[A\,,\,C] = 0$.

"It follows that $[B\,,\,C] = 0$."

(f) "The energy spectrum of a quantum mechanical particle moving under the influence of an arbitrary potential must necessarily be either wholly discrete, or wholly continuous, but not partially discrete and partially continuous."

(g) "The existence of operators that commute with the Hamiltonian of a system generally implies that the energy spectrum of the system is degenerate."

(h) "The expectation value of the kinetic energy of a quantum mechanical particle can never be negative."

(i) Let A and B be the operators corresponding to two physical observables of a system.

"If A and B do not commute with each other, then the product of uncertainties in these two quantities can never be zero in any state of the system."

(j) "The eigenvalues of the operator corresponding to a physical observable of a system are the only possible results of a measurement of that observable."

2. Fill in the blanks.

(a) The Hamiltonian of a particle moving in one dimension is given by $H = p^2/(2m) + V(x)$ where x and p denote the position and momentum operators. Then the double commutator $\big[x\,,\,[x\,,\,H]\big] = \cdots$

(b) A system can have two possible states, denoted by $|1\rangle$ and $|2\rangle$, respectively. These states are normalized, and mutually orthogonal. The Hamiltonian of the system is given by

$$H = a\Big(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\Big),$$

where a is a real constant. In the basis formed by the states $|1\rangle$ and $|2\rangle$, H is represented by the matrix $\cdots$

(c) A particle moving in one dimension is in a state $|\Psi\rangle$. Its position-space wave function is given by $\langle x|\Psi\rangle \equiv \psi(x)$. Consider the state $|\Phi\rangle = e^{i\,a\,p}\,|\Psi\rangle$ where a is a real constant and p is the momentum operator of the particle. The position-space wave function in the state $|\Phi\rangle$ is then given by $\phi(x) = \cdots$

(d) Let $|\alpha\rangle$ be a normalized coherent state of the linear harmonic oscillator, so that $a\,|\alpha\rangle = \alpha\,|\alpha\rangle$. The expectation value of the number operator in this state is $\langle\alpha|a^\dagger\,a|\alpha\rangle = \cdots$

(e) The energy levels of an isotropic two-dimensional harmonic oscillator are given by $E(n_1\,,\,n_2) = \hbar\omega\,(n_1 + n_2 + 1)$, where n_1 and n_2 are non-negative integers. The degeneracy of the energy level $6\,\hbar\omega$ is $\cdots$

(f) The energy levels of an isotropic three-dimensional harmonic oscillator are given by $E(n) = \hbar\omega\left(n + \frac{3}{2}\right)$, where n runs over the non-negative integers. The degeneracy of the energy level E_n is $\cdots$

(g) The expectation value of the kinetic energy of a linear harmonic oscillator of mass m and frequency ω in the energy eigenstate $|n\rangle$ is $\cdots$

(h) The dependence of the energy E_n on the quantum number n for a particle moving in the potential kx^6 (where k is a positive constant) is $E_n \sim \cdots$

(i) The condition that an infinite sequence $(x_1\,,\,x_2\,,\,\ldots)$ be square-summable is $\cdots$

(j) If $[x\,,\,p] = i\hbar\,I$, then $[x\,,\,f(p)] = \cdots$

Fun with spin $\frac{1}{2}$

Rotations of the coordinate axes: In three-dimensional space, a general rotation of the coordinate axes about the origin can be completely specified by a unit vector $\mathbf{n}$ and an angle θ, where $0 \leq \theta \leq \pi$. The rotation occurs in the plane whose normal is $\mathbf{n}$, and θ is the angle through which the coordinate frame is rotated. We'll denote such a rotation by $R(\mathbf{n}, \theta)$.[15] The point is that $R(\mathbf{n}, \theta)$ is *represented* by different kinds of objects (e.g., matrices of different dimensions, differential operators, etc.), depending on the *sort* of quantity whose behaviour under the rotation we are interested in deducing.

Pauli matrices: As we have seen in class, an explicit representation of the angular momentum algebra in the case $j = \frac{1}{2}$ is provided by the Pauli matrices. Recall their definition,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Setting $J_i = \frac{1}{2}\hbar\,\sigma_i$, it is easy to verify that the angular momentum algebra $[J_i\,,\,J_j] = i\hbar\,\epsilon_{ijk}\,J_k$ is satisfied. That is, the matrices $\frac{1}{2}\hbar\,\sigma_i$ $(i = 1, 2, 3)$ provide a **representation** of the generators of rotations in three-dimensional space. As numerous problems, both in quantum mechanics as well as other contexts, can be reduced to 'two-level' problems, the Pauli matrices are of fundamental importance, and play a most useful role. Note the following basic properties of each of the Pauli matrices σ_i $(i = 1, 2, 3)$:

(i) σ_i is hermitian, traceless, with determinant equal to -1.

(ii) $\sigma_i^2 = I$, where I is the 2×2 unit matrix; hence $\sigma_i^{-1} = \sigma_i$.

(iii) σ_i has eigenvalues 1 and -1, with normalized eigenvectors $\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$ and $\left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$ respectively.

It is customary to denote the set of three matrices $(\sigma_1\,,\,\sigma_2\,,\,\sigma_3)$ by the 'vector' $\boldsymbol{\sigma}$. This is not just a matter of notation. We know that the angular momentum generators J_i themselves transform like the components of a vector under rotations of the coordinate axes (in three-dimensional space). Under a rotation $\mathbf{J}$ transforms according to

$$\mathbf{J}' = R(\mathbf{n}, \theta)\,\mathbf{J}\,R^\dagger(\mathbf{n}, \theta) = e^{i\mathbf{J}\cdot\mathbf{n}\,\theta}\,\mathbf{J}\,e^{-i\mathbf{J}\cdot\mathbf{n}\,\theta}.$$

Exactly the same transformation law applies to any other *vector* operator as well.

Here are some more properties of the Pauli matrices:

1. Find the matrices $e^{i\alpha\sigma_1}$, $e^{i\beta\sigma_2}$ and $e^{i\gamma\sigma_3}$, where $\alpha\,,\beta$ and γ are any three arbitrary complex numbers.

2. The basis formed by I and $\boldsymbol{\sigma}$: Show that an *arbitrary* 2×2 matrix $M = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ can be written as a linear combination of $I\,,\,\sigma_1\,,\,\sigma_2$ and σ_3 in a unique manner.

[15] You might wonder why the range of θ is $0 \leq \theta \leq \pi$, rather than $0 \leq \theta < 2\pi$. The reason is that 0 to π suffices to cover all possible rotations, because *a rotation about the direction* $\mathbf{n}$ *through an angle* π *is exactly the same as a rotation about the opposite direction* $-\mathbf{n}$ *through an angle* π. (Check it out!) This seemingly simple fact has truly profound consequences. It makes the parameter space of rotations (the space of all possible unit vectors $\mathbf{n}$ and all possible values of θ) have a nontrivial topology. In technical terms, it makes the parameter space *doubly-connected*. As a consequence, we have two distinct kinds of representations of the rotation group: the so-called tensor representations, and the so-called spinor representations. This leads, ultimately, to the existence of two kinds of elementary particles, namely, bosons and fermions.

In other words, M can be written as $\alpha_0\, I + \alpha_1\, \sigma_1 + \alpha_2\, \sigma_2 + \alpha_3\, \sigma_3$, where the elements $(a,\, b,\, c\,, d)$ uniquely determine the coefficients $(\alpha_0, \alpha_1,\, \alpha_2,\, \alpha_3)$, and vice versa. Note, in particular, that any *traceless* 2×2 matrix can be expanded uniquely as a linear combination of the three Pauli matrices.

3. Commutator and anticommutator: Show that $\sigma_k\, \sigma_l = i\, \epsilon_{klm}\, \sigma_m$, where the indices run over the values $1, 2$ and 3. Hence verify that

$$\sigma_k\, \sigma_l - \sigma_l\, \sigma_k \equiv [\sigma_k\,,\, \sigma_l] = 2\, i\, \epsilon_{klm}\, \sigma_m\,,$$

and that

$$\sigma_k\, \sigma_l + \sigma_l\, \sigma_k \equiv [\sigma_k\,,\, \sigma_l]_+ = 2\, \delta_{kl}\, I\,.$$

Therefore the commutator of any two different Pauli matrices is a constant times the third Pauli matrix, while the anticommutator of two different Pauli matrices is identically zero.

4. The exponential of a (2×2) **matrix**: Use the anticommuting property of the Pauli matrices to derive the following important relation. Let $\mathbf{a}$ be an ordinary vector with Cartesian components $(a_1\,,\, a_2\,,\, a_3)$, and let $\mathbf{a} \cdot \boldsymbol{\sigma}$ stand for the matrix $a_1\, \sigma_1 + a_2\, \sigma_2 + a_3\, \sigma_3$. Show that

$$\exp\,(i \mathbf{a} \cdot \boldsymbol{\sigma}) = I\, \cos\, a + i\, \frac{(\mathbf{a} \cdot \boldsymbol{\sigma})}{a}\, \sin\, a\,,$$

where $a = (a_1^2 + a_2^2 + a_3^2)^{1/2}$. This is the (2×2) matrix analog of the familiar Euler formula $e^{i\theta} = \cos\,\theta + i\, \sin\,\theta$ for an ordinary (real or complex) number θ.

The formula above is readily extended to the case of $\exp\,(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})$, where $\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}$ stands for $\alpha_1\, \sigma_1 + \alpha_2\, \sigma_2 + \alpha_3\, \sigma_3$, and $(\alpha_1\,,\, \alpha_2\,,\, \alpha_3)$ are real numbers. Simply set $i\, \mathbf{a} = \boldsymbol{\alpha}$, i.e., $a_1 = -i\, \alpha_1\,,\, a_2 = -i\, \alpha_2\,,\, a_3 = -i\, \alpha_3$ in the formula, to show that

$$\exp\,(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}) = I\, \cosh\, \alpha + \frac{(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})}{\alpha}\, \sinh\, \alpha\,,$$

where $\alpha = (\alpha_1^2 + \alpha_2^2 + \alpha_3^2)^{1/2}$. What has actually been done here is an *analytic continuation* of the original formula from real values of the quantities $(a_1\,,\, a_2\,,\, a_3)$ to pure imaginary values of these variables. Finally, since *any* 2×2 matrix M can be written in the form $M = \alpha_0\, I + \boldsymbol{\alpha} \cdot \boldsymbol{\sigma}$, we have

$$e^M = e^{\alpha_0} \Big\{ I\, \cosh\, \alpha + \frac{(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})}{\alpha}\, \sinh\, \alpha \Big\}.$$

5. Let $\mathbf{a}$ and $\mathbf{b}$ denote any two ordinary vectors, and $\mathbf{n}$ any unit vector. Establish the following identities:

(a) $(\mathbf{a} \cdot \boldsymbol{\sigma})\, (\mathbf{b} \cdot \boldsymbol{\sigma}) = (\mathbf{a} \cdot \mathbf{b})\, I + i\, (\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}$

(b) $[(\mathbf{a} \cdot \boldsymbol{\sigma})\,, (\mathbf{b} \cdot \boldsymbol{\sigma})] = 2i\, (\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}$

(c) $[\boldsymbol{\sigma}\,, (\mathbf{a} \cdot \boldsymbol{\sigma})] = 2i\, (\mathbf{a} \times \boldsymbol{\sigma})$

(d) $(\boldsymbol{\sigma} \times \mathbf{n})\, (\boldsymbol{\sigma} \cdot \mathbf{n}) = i \boldsymbol{\sigma} - i (\boldsymbol{\sigma} \cdot \mathbf{n})\, \mathbf{n}$

Note, incidentally, that the eigenvalues of $\boldsymbol{\sigma} \cdot \mathbf{n}$ remain equal to 1 and -1, for all unit vectors $\mathbf{n}$.

6. Let A be a self-adjoint operator with discrete eigenvalues λ_n , and let the corresponding normalized eigenfunctions $|\phi_n\rangle$ form a complete set in the Hilbert space. Then A can be written as

$$A = \sum_n \lambda_n \, P_n \quad \text{where} \quad P_n = |\phi_n\rangle\langle\phi_n|.$$

This is called the **spectral resolution** of the operator A.

(a) What is the spectral resolution of the operator $\mathbf{a} \cdot \boldsymbol{\sigma}$, where $\mathbf{a} = (a_1 \, , \, a_2 \, , \, a_3)$ is an ordinary vector?

The operator $R(z) = (A - zI)^{-1}$, where z is a complex variable, is called the **resolvent** of the operator A.

(b) Find the resolvent of the operator $\mathbf{a} \cdot \boldsymbol{\sigma}$. Where are the singularities of $R(z)$ located, in the complex z-plane?

The spin of a quantum mechanical particle is its *intrinsic* angular momentum.

- It is very important to realize that the spin of a particle is not connected to any mechanical motion of the particle, such as rotation about an axis. The spin of a particle is an intrinsic property of the particle, like its rest mass or its charge, if any.

The spin is present even in the rest frame of the particle, i.e., even when its linear momentum is zero. Like all angular momenta, the spin is also quantized. That is, if $\mathbf{S}$ denotes the spin operator of a particle (this is standard notation), then the operator $\mathbf{S}^2$ always has the eigenvalue $\hbar^2 S(S+1)$, where S is the spin quantum number of the particle. Each particle has a definite S. As in the case of all angular momenta, the possible values of S can only be $0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. Particles such as electrons, protons, neutrons, etc. have $S = \frac{1}{2}$, while photons have $S = 1$, pions have $S = 0$, and so on. Integer-spin particles are called **bosons**, while half-odd-integer-spin particles are called **fermions**. Any particular component $\mathbf{S} \cdot \mathbf{n}$ of a spin-S particle can only have $(2S+1)$ possible eigenvalues, given by $-\hbar S$, $-\hbar(S-1)$, $\ldots$, $\hbar(S-1)$, $\hbar S$. This is an equi-spaced sequence, with a spacing $\hbar$ between adjacent values. The 'spin-space' of a spin-S particle is thus a $(2S+1)$-dimensional linear vector space. The components of the spin operator $\mathbf{S}$ can thus be represented by $(2S+1) \times (2S+1)$ hermitian matrices, while the spin part of the state vector of the particle can be represented by a $(2S+1) \times 1$ column matrix in this space. Different components of the spin operator do not commute with each other.

What is the origin of the spin of a particle? At this level, the appropriate answer is that it is a consequence of quantum mechanics together with relativistic (or Lorentz) invariance.

- The rest mass and the spin of a quantum mechanical particle arise naturally when we impose the requirement that its state vector (or wave function) have a definite transformation property under **inhomogeneous Lorentz transformations**. The latter comprise **translations** of the origin of the space coordinates and of the time coordinate, **rotations** of the coordinate axes, and **boosts**[16] or velocity transformations from one inertial frame to another.

[16] These (alone) are called Lorentz transformations in elementary treatments, but it is preferable to avoid this confusing terminology.

As I have just said, the spin of a particle is a quantum mechanical property. (In fact, as just stated, it requires *relativistic* quantum mechanics, or more accurately, quantum field theory, to begin to understand its origin. In nonrelativistic quantum mechanics, the spin is "put in by hand".) As S is generally small for particles such as electrons, protons, atoms, etc., $\hbar S$ is infinitesimally small compared with the magnitudes of angular momenta that occur in rotational or orbital motion of macroscopic objects in daily life. For instance, a stone of mass $m = 1\,\mathrm{kg}$ tied to a string and twirled around in a circle of radius $r = 1\,\mathrm{m}$ with a time period of revolution equal to 1 s (or angular frequency $\omega = (2\pi)\ \mathrm{s}^{-1}$) has an orbital angular momentum of magnitude (2π) Js. But the angular momentum must be quantized, according to the rules of quantum mechanics. It is at once evident that the corresponding quantum number ℓ must be enormous in this instance: it must of of the order of 10^{+34}, so that the product $\hbar\ell$ is of the order of unity. This is why we don't see the quantization of angular momentum in daily life, when dealing with macroscopic objects. *The quantum numbers involved are so large compared with unity that the discreteness of the angular momentum is completely masked.* The classical limit may be obtained by letting $\hbar \to 0$ and $\ell \to \infty$, such that the product $\hbar\ell$ tends to the classical value of the magnitude of the angular momentum. In the case of spin, however, S is of the order of unity. Therefore there is no question of passing to a non-zero classical limit to obtain a finite value of $\hbar S$ in the limit $\hbar \to 0$. It is in this sense that one often comes across the statement, "Spin has no classical analog".

Now consider the spin operator of a 'spin-half' or $S = \frac{1}{2}$ particle like the electron. The spin space has $(2 \times \frac{1}{2} + 1) = 2$ dimensions in this case. The spin operator is most conveniently represented in this space in terms of the Pauli matrices, as

$$\mathbf{S} = \tfrac{1}{2}\hbar\,\boldsymbol{\sigma}.$$

Since $\boldsymbol{\sigma}\cdot\mathbf{n}$ (where $\mathbf{n}$ is a unit vector) has eigenvalues ± 1, this automatically ensures that $\mathbf{S}\cdot\mathbf{n}$ has eigenvalues $\pm\frac{1}{2}\hbar$, as required. As is clear from the very convention we have used for the Pauli matrices, it is customary to choose the 'axis of quantization' as the z-axis, so that S_z is represented by a diagonal matrix (and all other components are not). But you must remember that this is just a matter of convention, adopted unless explicitly stated otherwise.

We have seen that $\frac{1}{2}\hbar$ is indeed very small in magnitude by classical standards. How, then, can one detect it? It turns out that **intrinsic magnetic dipole moments** are generally associated with particles that have nonzero spin. This also requires that the particles be charged electrically, such as the electron, or at least have constituents that are charged, such as the neutron—which is electrically neutral, but is made up of three charged quarks. The intrinsic magnetic dipole moment of a particle of charge e and rest mass m is related to its spin by

$$\boldsymbol{\mu} = \frac{ge}{2m}\,\mathbf{S},$$

where g is called the g-factor of the particle. For spin-$\frac{1}{2}$ particles, relativistic quantum mechanics leads to the result $g = 2$. However, **quantum field theory** yields corrections to this result. The contribution from $g - 2$ to the intrinsic magnetic moment is called the **anomalous magnetic moment** of the particle concerned. This correction can be small compared to unity (as in the case of the electron), or indeed of the order of unity itself (as in the case of the proton and neutron). Let us consider the electron, as this is the relevant case for most applications in condensed matter physics. Taking $g = 2$ (which is adequate for most practical purposes), the

intrinsic magnetic moment of the electron is given by[17]

$$\boldsymbol{\mu}_e = \frac{ge}{2m_e}\,\mathbf{S} = -\frac{2|e|}{2m_e}\frac{\hbar}{2}\,\boldsymbol{\sigma} = -\frac{|e|\hbar}{2m_e}\boldsymbol{\sigma},$$

where $|e|$ is the magnitude of the electronic charge, and m_e is the rest mass of the electron. Hence the eigenvalues of any component of $\boldsymbol{\mu}$ are $\pm|e|\hbar/(2m_e)$. The quantity $|e|\hbar/(2m_e) \equiv \mu_B$ should be familiar to you as the **Bohr magneton**. Thus

$$\boldsymbol{\mu}_e = -\mu_B\,\boldsymbol{\sigma}.$$

The intrinsic magnetic moment of the electron gives us a way of probing its spin states. In an applied magnetic field $\mathbf{B}$, the Hamiltonian of the electron has an additional term $-\boldsymbol{\mu}_e\cdot\mathbf{B}$. This leads to a torque on the dipole. If the field is also spatially nonuniform, there is also a force on the dipole. This is the basis of the famous and pivotal **Stern-Gerlach experiment** which originally demonstrated the existence of spin.

Spin-$\frac{1}{2}$ states and operators: In what follows, we assume that the basis for the spin states of an electron is one in which S_z is diagonal. We shall use the convenient notation

$$|\uparrow\rangle \stackrel{\text{def.}}{=} |S=\tfrac{1}{2}\,,\,m=\tfrac{1}{2}\rangle\,,\ |\downarrow\rangle \stackrel{\text{def.}}{=} |S=\tfrac{1}{2}\,,\,m=-\tfrac{1}{2}\rangle\,.$$

Orthonormalization implies that

$$\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1,\ \langle\uparrow|\downarrow\rangle = \langle\downarrow|\uparrow\rangle = 0.$$

It follows that any arbitrary, normalized, time-dependent spin state of the electron can be written in the form

$$|\Psi(t)\rangle = a(t)\,|\uparrow\rangle + b(t)\,|\downarrow\rangle\,,\quad \text{where}\quad |a(t)|^2 + |b(t)|^2 = 1.$$

Note that the natural representation in the spin space is

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

7. It is clear that the four operators $|\uparrow\rangle\langle\uparrow|\,,\ |\uparrow\rangle\langle\downarrow|\,,\ |\downarrow\rangle\langle\uparrow|$ and $|\downarrow\rangle\langle\downarrow|$ form a basis for all *operators* acting on the spin states of an electron. Write down the operators

$$S_x\,,\ S_y\,,\ S_z\,,\ S_x^2\,,\ S_y^2\,,\ S_z^2\,,\ S_x\,S_y\,,\ S_y\,S_z\ \text{ and }\ S_z\,S_x$$

in this basis.

8. In the state $|\uparrow\rangle$, calculate the expectation values of $\langle S_x\rangle$ and $\langle S_y\rangle$, as well as $\langle S_x^2\rangle$ and $\langle S_y^2\rangle$. Hence find the uncertainty product $(\Delta S_x)\,(\Delta\,S_y)$, and verify that the uncertainty relation

$$(\Delta S_x)\,(\Delta\,S_y) \geq \tfrac{1}{2}\big|\langle\,[S_x\,,\,S_y]\,\rangle\big|$$

is satisfied. Repeat the calculation (or write down the answers!) for the state $|\downarrow\rangle$.

9. For a spin-$\frac{1}{2}$ particle, write down the commutator $[\mathbf{S}\cdot\mathbf{n}\,,\,\mathbf{S}\cdot\mathbf{n}']$, where $\mathbf{n}$ and $\mathbf{n}'$ are two arbitrary unit vectors. (Use the identity already established for the commutator $[(\mathbf{a}\cdot\boldsymbol{\sigma})\,,\,(\mathbf{b}\cdot\boldsymbol{\sigma})]$.)

[17] Note the appearance of several different factors of 2.

10. Precession of the spin in a magnetic field: Here is the simplest version of the effect of a magnetic field on the spin of an electron. Suppose the electron is prepared, with the help of a magnetic field in the z-direction, in the initial state $|\chi(0)\rangle = |\uparrow\rangle$. The field is switched off, and in its place a constant, uniform, *transverse* magnetic field $\mathbf{B} = B\,\mathbf{e}_x$ is applied. The (magnetic part of the) Hamiltonian is given by

$$H = -\boldsymbol{\mu}_e \cdot \mathbf{B} = \mu_B\,(\boldsymbol{\sigma} \cdot \mathbf{B}) = \mu_B\,B\,\sigma_1\,.$$

(a) Show that the spin state at any subsequent time t is given by

$$|\chi(t)\rangle = \left(\cos\,\tfrac{1}{2}\omega_c\,t\right)\,|\uparrow\rangle - \left(i\,\sin\,\tfrac{1}{2}\omega_c\,t\right)\,|\downarrow\rangle,$$

where $\omega_c = |e|B/m_e$ is the precession frequency.

(b) Hence sketch the probabilities $P_\uparrow(t)$ and $P_\downarrow(t)$ that the electron is in the 'spin up' state and the 'spin down' state, respectively, at time t.

This example should help you understand why we may regard a 'transverse' component of the spin operator (either S_x or, equivalently, σ_1) as a **spin flip operator**.

11. A generalization: A straightforward generalization of the case just considered is the following. Let the initial state of the electron be given by

$$|\chi(0)\rangle = a|\uparrow\rangle + b|\downarrow\rangle = \begin{pmatrix} a \\ b \end{pmatrix},$$

where a and b are given complex constants satisfying $|a|^2 + |b|^2 = 1$. It is clear that $|a|^2$ and $|b|^2$ represent the respective probabilities of obtaining the results $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$ in a measurement of the component S_z of the spin of the electron. Note that the expectation value of S_z in this state is

$$\langle\chi(0)\,|\,S_z\,|\,\chi(0)\rangle = \frac{1}{2}\hbar\,(|a|^2 - |b|^2).$$

In the presence of a magnetic field $\mathbf{B} = B\mathbf{n}$ where $\mathbf{n}$ is an arbitrary unit vector, the Hamiltonian is $H = \mu_B\,B\,(\boldsymbol{\sigma} \cdot \mathbf{n})$. Find the spin state $|\chi(t)\rangle$ for all $t > 0$. Find also the expectation value of S_z at time t.

Comparison with the precession of a classical dipole moment: Let us compare the behavior of the quantum mechanical magnetic moment (or spin) with that of a *classical* dipole moment $\boldsymbol{\mu}_{\rm cl}$ in a constant, uniform magnetic field $\mathbf{B}$.

A classical magnetic dipole moment is generated by a current loop. Consider a classical particle of charge e and mass m moving in a circular orbit of radius r with a time period T. The orbital angular momentum is given by $\mathbf{L} = mr^2\omega\mathbf{n}$, where $\omega = 2\pi/T$ is the angular speed of the particle and $\mathbf{n}$ is the unit normal to the plane of the orbit. The magnetic moment associated with the current loop has a magnitude equal to the area of the loop multiplied by the current, by Ampere's rule. Hence $\boldsymbol{\mu}_{\rm cl} = \pi r^2(e/T)\mathbf{n} = \frac{1}{2}er^2\omega\mathbf{n}$. The dipole experiences a torque $\boldsymbol{\mu}_{\rm cl} \times \mathbf{B}$ in the presence of the magnetic field. Equating this torque to the rate of change of angular momentum, we get the equation of motion

$$\frac{d\mathbf{L}}{dt} = \boldsymbol{\mu}_{\rm cl} \times \mathbf{B} = \frac{e}{2m}(\mathbf{L} \times \mathbf{B}).$$

The factor $e/(2m)$ is the **gyromagnetic ratio** in this case. It follows at once that the dipole moment executes *precessional motion* around the direction of the magnetic field, with an angular frequency (called the **Larmor frequency**) equal to

$|e|B/(2m)$.

12. Now consider the quantum mechanical counterpart of this problem. To be specific, consider the spin of an electron when it is placed in a magnetic field. As we have already found, the intrinsic magnetic moment operator of the electron may be written in the form $\boldsymbol{\mu}_e = -\mu_B\,\boldsymbol{\sigma}$, while the Hamiltonian is given by $H = -\boldsymbol{\mu}_e \cdot \mathbf{B} = \mu_B\,(\boldsymbol{\sigma}\cdot\mathbf{B})$. It is most convenient to work in the Heisenberg picture.

(a) Write down the Heisenberg equation of motion for the spin operator $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$.

(b) Use one of the identities established in the foregoing in connection with Pauli matrices, to show that the equaiton of motion simplifies to

$$\frac{d\mathbf{S}}{dt} = \frac{e}{m_e}\,(\mathbf{S}\times\mathbf{B}) = \boldsymbol{\mu}_e \times \mathbf{B}.$$

Note that this equation of motion is precisely of the *form* that is obtained in the classical case. Taking expectation values (in any arbitrary state of the electron) on both sides,

$$\frac{d\langle\mathbf{S}\rangle}{dt} = \langle\boldsymbol{\mu}_e\rangle \times \mathbf{B}.$$

Thus the *expectation values* of the angular momentum and the magnetic moment are related precisely as they are in the classical case. This is yet another instance of Ehrenfest's Theorem.

But there is a difference of a factor of 2 between the angular frequency of precession of the classical dipole $\boldsymbol{\mu}_{\rm cl}$ and the quantum mechanical expectation value $\langle\boldsymbol{\mu}_e\rangle$(!) The classical frequency of precession is $|e|B/(2m)$, while in the quantum mechanical case it is $|e|B/m_e$. Inspection shows that this difference arises as a result of the fact that the g-factor of the electron is equal to 2, so that the gyromagnetic ratio is now $ge/(2m_e) = e/m_e$ rather than $e/(2m)$. I have already mentioned that the result $g = 2$ follows from the relativistic quantum mechanics of an electron.

13. Consider the spin state

$$|\chi\rangle = a|\uparrow\rangle + b|\downarrow\rangle = \begin{pmatrix} a \\ b \end{pmatrix},$$

where a and b are given constants (complex numbers) satisfying $|a|^2 + |b|^2 = 1$. We know that $|a|^2$ and $|b|^2$ are the probabilities that a measurement of S_z will yield the result $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$ respectively. That is, they are the probabilities that the spin is 'up' or 'down' in the state $|\chi\rangle$.

(a) Show that the expectation values of the components S_x and S_y in the state $|\chi\rangle$ are given by

$$\langle S_x\rangle = \langle\chi\,|\,S_x\,|\,\chi\rangle = \hbar\,\mathrm{Re}\,(a^*b) \text{ and } \langle S_y\rangle = \langle\chi\,|\,S_y\,|\,\chi\rangle = \hbar\,\mathrm{Im}\,(a^*b),$$

respectively. Note that these expectation values vanish if either a or b is zero, as one might expect 'intuitively' (the spin is then 'oriented' along the z-axis!)

There is another way to regard the state $|\chi\rangle$. Suppose we measure the component $(\mathbf{S}\cdot\mathbf{n})$ of the spin of an electron along an arbitrary direction in space, given by the unit vector $\mathbf{n}$ with respect to our fixed coordinate system (in which S_z is represented by a diagonal matrix, etc.). Let the direction $\nearrow$ of the vector $\mathbf{n}$ be specified by the

spherical polar coordinates $(\theta\,,\,\varphi)$ in the fixed coordinate system. The result of the measurement will be either $\frac{1}{2}\hbar$ or $-\frac{1}{2}\hbar$. We could then say that, immediately after the measurement, the electron spin is either 'along' $\mathbf{n}$ or along $-\mathbf{n}$, respectively. Let us denote the corresponding states by $|\nearrow\rangle$ and $|\swarrow\rangle$, respectively.[18]

(b) Using the fact that the Cartesian components of $\mathbf{n}$ are given by

$$\mathbf{n} = (\sin\theta\,\cos\varphi\,,\,\sin\theta\,\sin\varphi\,,\,\cos\theta),$$

show that $|\nearrow\rangle$ can be represented as

$$|\nearrow\rangle = \begin{pmatrix} \cos\frac{1}{2}\theta \\ e^{-i\varphi}\,\sin\frac{1}{2}\theta \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} e^{i\varphi/2}\,\cos\frac{1}{2}\theta \\ e^{-i\varphi/2}\,\sin\frac{1}{2}\theta \end{pmatrix},$$

apart from an arbitrary overall multiplicative phase factor $e^{i\alpha}$.

The general state $\binom{a}{b}$ with $|a|^2 + |b|^2 = 1$ can thus be regarded as the 'up' state in terms of an 'axis of quantization' $\mathbf{n}$ that is different from the usual z-axis. The modulus of a can be regarded as the cosine of half the polar angle of $\mathbf{n}$, while that of b is the sine of this angle. The phase difference between the complex numbers a and b is just the azimuthal angle φ of the direction $\mathbf{n}$.

Since

$$\begin{aligned} -\mathbf{n} &= \big(\sin(\pi-\theta)\,\cos(\pi+\varphi)\,,\,\sin(\pi-\theta)\,\sin(\pi+\varphi)\,,\,\cos(\pi-\theta)\big) \\ &= (-\sin\theta\,\cos\varphi\,,\,-\sin\theta\,\sin\varphi\,,\,-\cos\theta), \end{aligned}$$

we find

$$|\swarrow\rangle = \begin{pmatrix} \sin\frac{1}{2}\theta \\ -e^{-i\varphi}\,\cos\frac{1}{2}\theta \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} e^{i\varphi/2}\,\sin\frac{1}{2}\theta \\ -e^{-i\varphi/2}\,\cos\frac{1}{2}\theta \end{pmatrix}.$$

(c) Use the result just found to show that the normalized 'up' and 'down' states, if we consider the x-axis to be the axis of quantization, are given by

$$|S_x = \tfrac{1}{2}\hbar\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad \text{and} \quad |S_x = -\tfrac{1}{2}\hbar\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}.$$

(You have only to note that the positive x-direction corresponds to $\theta = \frac{1}{2}\pi\,,\,\varphi = 0$, while the negative x-direction corresponds to $\theta = \frac{1}{2}\pi\,,\,\varphi = \pi$.)

(d) Similarly, if the y-axis is taken to be the axis of quantization, show that the 'up' and 'down' states are given by

$$|S_y = \tfrac{1}{2}\hbar\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} \quad \text{and} \quad |S_y = -\tfrac{1}{2}\hbar\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}.$$

(e) Let's return to the general state $|\chi\rangle = \binom{a}{b}$, with $|a|^2 + |b|^2 = 1$ as usual. Suppose we measure the component S_x when the electron is in the state $|\chi\rangle$. Show that the probabilities of obtaining the values $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$, respectively, are given by

$$\tfrac{1}{2}\,|a+b|^2 \quad \text{and} \quad \tfrac{1}{2}\,|a-b|^2.$$

Hint: Expand $|\chi\rangle$ in a linear combination of the basis states $|S_x = \frac{1}{2}\hbar\rangle$ and $|S_x = -\frac{1}{2}\hbar\rangle$. The square of the modulus of each coefficient gives the probability required.

[18] Three cheers for the power of LaTex!

Note that if

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \cos \frac{1}{2}\theta \\ e^{-i\varphi} \sin \frac{1}{2}\theta \end{pmatrix},$$

then these probabilities become

$$\tfrac{1}{2}\,(1 + \sin\,\theta\,\cos\,\varphi) \quad \text{and} \quad \tfrac{1}{2}\,(1 - \sin\,\theta\,\cos\,\varphi),$$

respectively. It is easily checked that these values reduce correctly to 1 and 0, respectively, when $\theta = \frac{1}{2}\pi\,,\ \varphi = 0$ (that is, when the state $|\chi\rangle$ is just the state $|S_x = \frac{1}{2}\hbar\rangle$ itself). Similarly, they reduce correctly to 0 and 1, respectively, when $\theta = \frac{1}{2}\pi\,,\ \varphi = \pi$ (that is, when the state $|\chi\rangle$ is just the state $|S_x = -\frac{1}{2}\hbar\rangle$ itself).

(f) Suppose we measure the component S_y when the electron is in the state $|\chi\rangle$ defined in the preceding part. Show that the probabilities of obtaining the values $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$, respectively, are given by

$$\tfrac{1}{2}\,|a + ib|^2 = \tfrac{1}{2}\,(1 + \sin\,\theta\,\sin\,\varphi) \quad \text{and} \quad \tfrac{1}{2}\,|a - ib|^2 = \tfrac{1}{2}\,(1 - \sin\,\theta\,\sin\,\varphi).$$

Once again, these expressions reduce correctly to the values 1 and 0 for $\theta = \frac{1}{2}\pi\,,\ \varphi = \frac{1}{2}\pi$ (that is, when the state $|\chi\rangle = |S_y = \frac{1}{2}\hbar\rangle$); and to the values 0 and 1, for $\theta = \frac{1}{2}\pi\,,\ \varphi = \frac{3}{2}\pi$ (that is, when the state $|\chi\rangle = |S_y = -\frac{1}{2}\hbar\rangle$).

14. Let S be the spin quantum number of a certain particle. Consider a system of two such particles, and let $\mathbf{S}_1$ and $\mathbf{S}_2$ be their spin operators. All the components of $\mathbf{S}_1$ commute with those of $\mathbf{S}_2$.

Show that the eigenvalues of the operator $(\mathbf{S}_1 \cdot \mathbf{S}_2)$ are given by $\frac{1}{2}\hbar^2\,[j(j+1) - 2S(S+1)]$, where j runs over the values $0, 1, 2, \ldots, 2S$ in steps of unity. Hence $(\mathbf{S}_1 \cdot \mathbf{S}_2)$ has $(2S+1)$ possible eigenvalues. The smallest eigenvalue is $-\hbar^2\,S(S+1)$, and the largest is $\hbar^2\,S^2$.

Orbital angular momentum

1. The operator corresponding to the orbital angular momentum of a particle about the origin of coordinates is defined as $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, where $\mathbf{r}$ and $\mathbf{p}$ are its position and linear momentum operators, respectively. The Cartesian components of $\mathbf{L}$ are $L_i = \epsilon_{ijk}\, x_j\, p_k$, where the indices run over the values 1, 2, 3. Note that we don't need to worry about the noncommutativity of x_i and p_i in defining the operator $\mathbf{L}$, since the cross product $\mathbf{r} \times \mathbf{p}$ never involves a product of the *same* component of the position and the momentum. The components of $\mathbf{L}$ satisfy the angular momentum algebra $[L_i\,,\, L_j] = i\hbar\, \epsilon_{ijk}\, L_k$.[19]

(a) Find the commutators $[L_i\,,\, x_j]$ and $[L_i\,,\, p_j]$.

(b) It is clear that, classically, all the quantities $\mathbf{r} \cdot \mathbf{L},\ \mathbf{L} \cdot \mathbf{r},\ \mathbf{p} \cdot \mathbf{L}$ and $\mathbf{L} \cdot \mathbf{p}$ vanish identically. This follows from the vector identity $\mathbf{a} \cdot (\mathbf{a} \times \mathbf{b}) = 0$ and the fact that $\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{a}$. But these identities are not necessarily true in the case of non-commuting operators that happen to be vectors as well. Show, however, that the corresponding quantum mechanical *operators* $\mathbf{r} \cdot \mathbf{L},\ \mathbf{L} \cdot \mathbf{r},\ \mathbf{p} \cdot \mathbf{L}$ and $\mathbf{L} \cdot \mathbf{p}$ also vanish identically.

(c) Show that

$$(\mathbf{L} \times \mathbf{r}) + (\mathbf{r} \times \mathbf{L}) = 2i\hbar\, \mathbf{r}.$$

(d) Suppose an operator A commutes with both L_x and L_y . Find the commutator $[A\,,\, L_z]$. (*Hint*: Use the Jacobi identity.)

As you know, the eigenvalues of $\mathbf{L}^2$ are given by $\hbar^2\, l(l+1)$, where the allowed values of the orbital angular momentum quantum number are $l = 0, 1, 2, \ldots$. For a given value of l, the eigenvalues of any one component of $\mathbf{L}$ (along any arbitrary direction, conventionally taken to be the z-direction) are given by $\hbar\, m$, where the 'magnetic quantum number' m can take on the $(2l + 1)$ possible values from $-l$ to l in steps of unity. The corresponding set of common eigenstates of $\mathbf{L}^2$ and L_z, denoted by $|\, l, m\rangle$, form a basis set of angular momentum states. We have

$$\mathbf{L}^2\, |\, l, m\rangle = \hbar^2 l(l+1)\, |\, l, m\rangle, \quad L_z\, |\, l, m\rangle = \hbar m\, |\, l, m\rangle.$$

For every given l,

$$\langle\, l, m\, |\, l, m'\,\rangle = \delta_{mm'}\ .$$

The raising and lowering operators $L_\pm$ are defined as $L_+ = L_x + iL_y$ and $L_- = L_x - iL_y$, respectively. In terms of these operators, the angular momentum algebra of commutators reads

$$[L_+\,,\, L_-] = 2\hbar\, L_z\,, \quad [L_z\,,\, L_+] = \hbar\, L_+\,, \quad [L_z\,,\, L_-] = -\hbar\, L_-\ .$$

It is clear that $L_+\, |l, l\rangle = 0$ and $L_-\, |l, -l\rangle = 0$.

(e) Show that

$$L_\pm\, |\, l, m\rangle = \hbar\, \sqrt{l(l+1) - m(m \pm 1)}\ |l, m \pm 1\rangle.$$

[19] This set of relations is sometimes written in the form $\mathbf{L} \times \mathbf{L} = i\hbar\mathbf{L}$, where we must remember that $\mathbf{L}$ stands for a set of three noncommuting operators, rather than an ordinary vector. Nothing is gained by this 'formula', as the proper version $[L_i\,,\, L_j] = i\hbar\epsilon_{ijk}\, L_k$ is just as compact.

It is also useful to note that

$$L_+ L_- = L_x^2 + L_y^2 + \hbar L_z = \mathbf{L}^2 - L_z^2 + \hbar L_z \,.$$

Similarly,

$$L_- L_+ = L_x^2 + L_y^2 - \hbar L_z = \mathbf{L}^2 - L_z^2 - \hbar L_z \,.$$

Hence the (basis) set of eigenstates of $\mathbf{L}^2$ and L_z is also the set of eigenstates of $L_+ L_-$ and $L_- L_+$. (That is, the operators $\mathbf{L}^2$, L_z, $L_+ L_-$ and $L_- L_+$ can be diagonalized simultaneously.)

2. Representation in position space: In position space, the Cartesian components of $\mathbf{L}$ are represented, of course, by the differential operators

$$L_x = y\,\frac{\partial}{\partial z} - z\,\frac{\partial}{\partial y}\,, \quad L_y = z\,\frac{\partial}{\partial x} - x\,\frac{\partial}{\partial z}\,, \quad L_z = x\,\frac{\partial}{\partial y} - y\,\frac{\partial}{\partial x}\,.$$

In spherical polar coordinates, these components are represented by the differential operators

$$\left.\begin{aligned} L_x &= i\hbar\Big(\sin\varphi\,\frac{\partial}{\partial\theta} + \cot\theta\,\cos\varphi\,\frac{\partial}{\partial\varphi}\Big), \\ L_y &= i\hbar\Big(-\cos\varphi\,\frac{\partial}{\partial\theta} + \cot\theta\,\sin\varphi\,\frac{\partial}{\partial\varphi}\Big), \\ L_z &= -i\hbar\,\frac{\partial}{\partial\varphi}\,. \end{aligned}\right\}$$

Hence the raising and lowering operators are represented in spherical polar coordinates by

$$\left.\begin{aligned} L_+ = L_x + i\,L_y &= \hbar\,e^{i\varphi}\Big(\frac{\partial}{\partial\theta} + i\,\cot\theta\,\frac{\partial}{\partial\varphi}\Big), \\ L_- = L_x - i\,L_y &= \hbar\,e^{-i\varphi}\Big(-\frac{\partial}{\partial\theta} + i\,\cot\theta\,\frac{\partial}{\partial\varphi}\Big). \end{aligned}\right\}$$

Verify that these operators, when acting on any (differentiable) function $f(\theta,\varphi)$ of the angular coordinates, satisfy the commutation relations given earlier.

The square of the total angular momentum is of course represented by a multiple of the angular part of the Laplacian,

$$\mathbf{L}^2 = -\hbar^2\Big[\frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\Big(\sin\theta\,\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\varphi^2}\Big].$$

Spherical harmonics: The position-space representatives (or wave functions) corresponding to the angular momentum eigenstates $|\,l,m\rangle$ are called **spherical harmonics**, and are denoted by $Y_{lm}(\theta,\varphi)$. Thus

$$Y_{lm}(\theta,\varphi) \stackrel{\text{def.}}{=} \langle\mathbf{n}\,|\,l,m\rangle \equiv \langle\theta,\varphi\,|\,l,m\rangle,$$

where the direction in space represented by the unit vector $\mathbf{n}$ is specified by the polar angle θ and azimuthal angle φ. The spherical harmonics are related to the Legendre polynomials as follows. Recall that the Legendre polynomial $P_l(\cos\theta)$ of order l is given by the Rodrigues formula (denoting $\cos\theta$ by ξ, say)

$$P_l(\xi) = \frac{1}{2^l\,l!}\,\frac{d^l}{d\xi^l}\,(\xi^2-1)^l.$$

The associated Legendre polynomial $P_l^m(\cos\theta)$ is defined (for $m \geq 0$) as

$$P_l^m(\xi) = (1-\xi^2)^{m/2}\,\frac{d^m}{d\xi^m}\,P_l(\xi) = \frac{1}{2^l\,l!}\,(1-\xi^2)^{m/2}\,\frac{d^{l+m}}{d\xi^{l+m}}\,(\xi^2-1)^l\,.$$

Note that $P_l^0(\cos\theta) \equiv P_l(\cos\theta)$. The spherical harmonic $Y_{lm}(\theta,\varphi)$ is then defined as

$$Y_{lm}(\theta,\varphi) = \sqrt{\frac{(2l+1)}{4\pi}\,\frac{(l-m)!}{(l+m)!}}\;P_l^m\,(\cos\theta)\,e^{im\varphi}.$$

For $m < 0$, the spherical harmonics are given by

$$Y_{l,-m}(\theta,\varphi) = (-1)^m\,Y_{lm}^*(\theta,\varphi),$$

where (as usual) the asterisk denotes complex conjugation. That is, for $m \geq 0$,

$$Y_{l,-m}(\theta,\varphi) = (-1)^m\,\sqrt{\frac{(2l+1)}{4\pi}\,\frac{(l-m)!}{(l+m)!}}\,P_l^m\,(\cos\theta)\,e^{-im\varphi}.$$

We have

$$\mathbf{L}^2\,Y_{lm}(\theta,\varphi) = \hbar^2\,l(l+1)\,Y_{lm}(\theta,\varphi) \quad \text{and} \quad L_z\,Y_{lm}(\theta,\varphi) = \hbar\,m\,Y_{lm}(\theta,\varphi),$$

where $\mathbf{L}^2$ and L_z are the respective differential operators given above. The orthonormality relation for the spherical harmonics is

$$\int d\Omega\,Y_{lm}^*(\theta,\varphi)\,Y_{l'\,m'}(\theta,\varphi) = \delta_{ll'}\,\delta_{mm'}$$

where $d\Omega = \sin\theta\,d\theta\,d\varphi$ is the solid angle element, and the integration is over all solid angles. The completeness relation is

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}^*(\theta,\varphi)\,Y_{lm}(\theta',\varphi') = \delta(\Omega-\Omega') = \frac{1}{\sin\theta}\,\delta(\theta-\theta')\,\delta(\varphi-\varphi').$$

3. Show explicitly (from the corresponding differential operator representations) that the action of the raising and lowering operators is given by

$$L_\pm\,Y_{lm}(\theta,\varphi) = \hbar\,\sqrt{l(l+1)-m(m\pm1)}\;Y_{l,m\pm1}(\theta,\varphi).$$

4. The Hamiltonian of a particle of mass m moving in a central potential $V(r)$ is

$$H = \frac{\mathbf{p}^2}{2m} + V(r).$$

(a) Show that the commutators $[L_i\,,\,p^2] = 0$ and $[L_i\,,\,r^2] = 0$, where $p^2 = \mathbf{p}\cdot\mathbf{p} = p_i\,p_i$ and $r^2 = \mathbf{r}\cdot\mathbf{r} = x_i\,x_i$.

(b) Hence show that $[L_i\,,\,H] = 0$.

(c) Use the position-space representation $p_i = -i\hbar\,\partial/\partial x_i$ of the linear momentum operator to show that

$$[p_i\,,\,r^{-1}] = i\hbar\,r^{-3}\,x_i\,.$$

(d) Hence write down the commutator $[p_i\,,\,H]$ in the case of the Coulomb potential $V(r) = -K/r$, where K is a constant.

5. The radial momentum operator: Classically, the radial momentum of a particle is simply the component of its linear momentum in the direction of its position vector, i.e., $p_r = \mathbf{e}_r \cdot \mathbf{p} = \mathbf{p} \cdot \mathbf{e}_r$, where $\mathbf{e}_r = \mathbf{r}/r$. Quantum mechanically, we must take into account the fact that $\mathbf{e}_r$ and $\mathbf{p}$ do not commute with each other. The radial momentum operator must be defined as

$$p_r \stackrel{\text{def.}}{=} \frac{1}{2}\Big(\mathbf{p} \cdot \frac{\mathbf{r}}{r} + \frac{\mathbf{r}}{r} \cdot \mathbf{p}\Big),$$

which ensures that p_r is a hermitian operator.

(a) Using the fact that $\mathbf{p}$ is represented by the differential operator $-i\hbar\nabla$ in the position representation, show that p_r is represented by the differential operator

$$p_r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right).$$

(b) Hence find the differential operator that represents p_r^2.

TEST

1. Are the statements in quotation marks true or false?

(a) "The state vector $|\Psi(t)\rangle$ of a quantum mechanical system with a hermitian Hamiltonian is obtained by a unitary transformation of its initial state vector $|\Psi(0)\rangle$."

(b) "No eigenstate of the position operator x of a quantum mechanical particle can be an eigenstate of the linear momentum p_x of the particle."

(c) "If $\mathbf{r}$ and $\mathbf{p}$ denote the position and linear momentum operators of a particle, then the operator $(\mathbf{r}\cdot\mathbf{p})$ commutes with the orbital angular momentum operator $\mathbf{L}=\mathbf{r}\times\mathbf{p}$."

(d) A particle of mass m moves in the one-dimensional potential well

$$V(x)=\begin{cases} -V_0 & \text{for} \quad 0<x<L \\ 0 & \text{for all other } x. \end{cases}$$

"There exists at least one bound state of the particle for all positive values of V_0 and L."

(e) A particle moves in three dimensions in a general attractive central potential $V(r)$.

"The energy eigenvalue of any bound state depends only on the principal quantum number n, and not on the orbital angular momentum quantum number l and the magnetic quantum number m."

(f) The Hamiltonian of a particle of mass m moving in three dimensions in an attractive Coulomb potential is given by

$$H=\frac{\mathbf{p}^2}{2m}-\frac{K}{r}\,, \quad (K>0).$$

"Then, if $\mathbf{A}=(\mathbf{p}\times\mathbf{L})-mK\mathbf{r}/r$, we have $[\mathbf{A}\,,\,H]=0$."

(g) The operators a, its adjoint $a^\dagger$, and the unit operator I satisfy the algebra $[a,I]=[a^\dagger,I]=0,\ [a,a^\dagger]=I$.

"There are no normalizable eigenstates of the operator $a^\dagger$."

(h) Consider the bound states of a particle moving in space under the influence of a central potential $V(r)$.

"In general, for a given value of the principal quantum number n, the energy eigenvalue of a bound state increases as the orbital angular momentum quantum number l increases."

(i) Let $|\uparrow\rangle$ and $|\downarrow\rangle$ denote the normalized eigenstates of S_z of a spin-half particle, corresponding to the eigenvalues $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$, respectively.

"The expectation value of S_x is zero in every state that is a linear combination of $|\uparrow\rangle$ and $|\downarrow\rangle$."

(j) "The normalized state $\big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\big)/\sqrt{2}$ corresponds to the singlet spin state of a two-electron system."

(k) A particle of mass m moving from left to right on the x-axis is incident upon a potential barrier given by

$$V(x) = \begin{cases} V_0 & \text{for} \quad 0 < x < L \\ 0 & \text{for all other } x, \end{cases}$$

where V_0 is a positive constant.

"If the energy E of the incident particle is greater than V_0, the reflection and transmission coefficients of the particle are given by $R = 0$ and $T = 1$, respectively."

(l) A Hamiltonian H_0 has discrete, non-degenerate eigenvalues $E_0^{(0)} < E_1^{(0)} < E_2^{(0)} < \ldots$. The Hamiltonian is perturbed, so that the new Hamiltonian is $H = H_0 + \lambda H'$, where λ is a real constant. The new energy levels are given by $E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} +$ terms of higher order in λ.

"The coefficient $E_0^{(2)}$ can never be positive."

(m) In the linear vector space ℓ_2 of square-summable sequences, consider the operator A whose action on any vector is given by

$$A\,(x_1\,,\,x_2\,,\,x_3\,,\,\ldots) = (0\,,\,x_1\,,\,x_2\,,\,\ldots).$$

"A is a linear operator with norm $\|A\| = 1$."

(n) "If the position-space wave function of a particle is normalized such that $\int |\psi(\mathbf{r},t)|^2\, d^3r = 1$ for all t, then its momentum-space wave function is also automatically normalized such that $\int |\widetilde{\psi}(\mathbf{p},t)|^2\, d^3p = 1$ for all t."

(o) Consider a perturbed Hamiltonian $H = H_0 + \lambda H'(t)$.

"In the interaction picture, the time evolution of the state vector of the system is governed by the unperturbed Hamiltonian H_0, while that of observables is governed by the perturbation $\lambda H'(t)$."

(p) "In the limit of large quantum number $n\,(\gg 1)$, the energy levels of a particle moving in the potential $V(x) = K\,|x|$ (where K is a positive constant) become approximately equally-spaced."

(q) Let A be a linear self-adjoint operator acting on the state vectors of a Hilbert space $\mathcal{H}$, and let the domain and range of A be $\mathcal{H}$ itself.

"If all the eigenvalues of A are finite in magnitude, we may conclude that A is a bounded operator, i. e., that its norm is finite."

(r) We know that the set of functions

$$\phi_n(x) = \frac{1}{\pi^{1/4}} \frac{1}{\sqrt{2^n\, n!}} e^{-x^2/2}\, H_n(x),$$

where $H_n(x)$ is the Hermite polynomial of order n, forms an orthonormal basis in the space $\mathcal{L}_2(-\infty\,,\,\infty)$.

"The set of functions $\phi_n(x)$ with $n = 1, 3, 5, \ldots$ forms an orthogonal basis in the space $\mathcal{L}_2(0\,,\,\infty)$."

(s) The Hamiltonian of a particle of mass m and charge e placed in a uniform, constant applied magnetic field is

$$H = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m}\,,$$

where $\mathbf{A}$ is the vector potential.

"Since the vector potential is dependent on the gauge we choose, the energy levels of the particle are also gauge-dependent."

(t) Continuation of the preceding question:

"In the presence of a magnetic field, the different Cartesian components of the momentum $\mathbf{p}$ of the particle commute with each other, but the different Cartesian components of its velocity $\mathbf{v} = d\mathbf{r}/dt$ do not commute with each other. "

(u) Consider a system with a hermitian but time-dependent Hamiltonian $H(t)$.

"Even though the Hamiltonian is time-dependent, the state vector $|\Psi\,(t)\rangle$ at any time $t > 0$ is given by a unitary transformation applied to the initial state vector $|\Psi\,(0)\rangle$."

(v) Consider a particle of mass m in a one-dimensional box: $V(x) = 0$ for $0 < x < L$, and infinite for all other x. Let E_1 denote the ground state energy of the particle. A potential $V(x) = \lambda\,\delta(x - \frac{1}{2}L)$ (where λ is a positive constant) is now switched on inside the box.

"The ground state energy of the particle will now be greater than E_1 ."

(w) "Proper rotations of the coordinate axes in three-dimensional space can be represented by (2×2) matrices that are unitary, and have determinant equal to unity."

(x) "The ground state of an electron in a hydrogen atom (the state with quantum numbers $n = 1,\ l = 0,\ m = 0$) is a minimum uncertainty state."

2. Fill in the blanks in the following.

(a) In the space $\mathcal{L}_2(-\infty\,,\,\infty)$ of square-integrable functions of a real variable x, the adjoints of the operators x^n and d^n/dx^n (where n is a positive integer) are $\cdots$ and $\cdots$

(b) Let p_r denote the radial momentum operator of a particle moving in three dimensions. Then, in the position basis, the operator p_r^2 is represented by the differential operator $-\hbar^2\left(\partial^2/\partial r^2 + A\right)$, where $A = \cdots$

(c) Let $\mathbf{S}_1$ and $\mathbf{S}_2$ be the spin operators of two independent spin-$\frac{1}{2}$ particles. The two possible eigenvalues of the operator $(\mathbf{S}_1 \cdot \mathbf{S}_2)/\hbar^2$ are then $\cdots$ and $\cdots$

(d) Let α and β be two normalized coherent states of the linear harmonic oscillator, where α and β are arbitrary complex numbers. Then $|\langle\alpha\,|\,\beta\rangle|^2 = \cdots$

(e) If $|\Psi\rangle$ is a normalized state vector of a system, the possible eigenvalues of the projection operator $|\Psi\rangle\langle\Psi|$ are $\cdots$ and $\cdots$

(f) The normalized probability that there are n photons of a given frequency ν and given polarization in blackbody radiation contained in a cavity at absolute temperature T is given by

$$P(n) = \frac{1}{\overline{n}+1}\Big(\frac{\overline{n}}{\overline{n}+1}\Big)^n, \quad \text{where} \quad \overline{n} = (e^{h\nu/k_BT} - 1)^{-1}\,.$$

In terms of $\overline{n}$, the variance of n is equal to $\cdots$

(g) Let $|\,j_1\,,\,m_1\,\rangle$ and $|\,j_2\,,\,m_2\,\rangle$ be the respective normalized angular momentum eigenstates of two particles with given angular momentum quantum numbers j_1 and j_2. We write the angular momentum eigenstates of the total system as

$$|\,j_1\,,\,m_1\,\rangle \otimes |\,j_2\,,\,m_2\,\rangle \equiv |\,j_1\,,\,j_2\,;\,m_1\,,\,m_2\,\rangle.$$

These are common eigenstates of the mutually commuting set of operators $J_1^2\,,\ J_{1z}\,,\ J_2^2$ and J_{2z}. Call this set of states basis I.

Adding the angular momenta, let $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$, and let m denote the quantum number corresponding to J_z. We may then work in terms of the alternative set of states $|\,j_1\,,\,j_2\,;\,j\,,\,m\,\rangle$. Call this basis II. These states are common eigenstates of the mutually commuting set of operators $\cdots$

(h) Continuing the preceding question, the basis-I states $|\, j_1\,,\, j_2\,;\, j_1\,,\, j_2\,\rangle$ and $|\, j_1\,,\, j_2\,;\, -j_1\,,\, -j_2\,\rangle$ must be the same as the basis-II states $\cdots$ and $\cdots$ respectively. (You must specify the values of j and m in writing down the corresponding $|\, j_1\,,\, j_2\,;\, j\,,\, m\,\rangle$ states.)

(i) Continuing further, the orthonormality relation for basis-II states is $\cdots$

(j) Finally, suppose $j_1 = j_2 = \frac{1}{2}$. Then the basis-II state $|\, \frac{1}{2}\,,\, \frac{1}{2}\,;\, 0\,,\, 0\,\rangle$, when written as a superposition of basis-I states, is given by $\cdots$

(k) Consider the oscillator raising and lowering operators satisfying the commutation relation $[a\,,\, a^\dagger] = I$. In the basis formed by the eigenstates $|n\rangle$ of $a^\dagger\, a$, operators are represented by infinite-dimensional matrices. The general matrix element of the operator a is given by $a_{ij} = \cdots$ where i and j run over the values $0, 1, 2, \ldots$ *ad inf.* (You must use appropriate Kronecker deltas to write down an expression for a_{ij} .)

(l) A spin-half particle is in the state $|\uparrow\rangle = \binom{1}{0}$ that is an eigenstate of S_z with eigenvalue $\frac{1}{2}\hbar$. Let $|\rightarrow\rangle$ and $|\leftarrow\rangle$ denote eigenstates of S_x corresponding to the eigenvalues $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$, respectively. The expansion of $|\uparrow\rangle$ in terms of these two eigenstates is $|\uparrow\rangle = \cdots$

(m) The Hamiltonian of a perturbed linear harmonic oscillator is given by

$$H = H_0 + \lambda H' = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + \frac{1}{4}\lambda x^4,$$

where λ is a small positive constant. The eigenvalue E_n of H is, correct to first order in λ, $E_n = \cdots$

(n) The Schrödinger equation for the position-space wave function $\psi(\mathbf{r}, t)$ of a particle of mass m moving in a potential $V(\mathbf{r})$ is

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi + V(\mathbf{r})\psi.$$

The wave function satisfies the continuity equation $\partial\rho/\partial t + \nabla \cdot \mathbf{j} = 0$, where $\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$, and the probability current density is given by $\mathbf{j}(\mathbf{r}, t) = \cdots$

(o) Continuing the preceding question, if the wave function has the asymptotic form (for very large values of r)

$$\psi(\mathbf{r}, t) = \frac{A}{r} e^{ikr}\, e^{-iEt/\hbar},$$

where A is a normalization constant, and k and E are positive constants, then $\mathbf{j}(\mathbf{r}, t) = \cdots$

(p) The Hamiltonian of a particle moving in one dimension is

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

Then $\big[x\,,\,[x\,,\,H]\,\big] = \cdots$

(q) Continuing with the preceding question: assume that the spectrum $\{E_n\}$ of H is discrete and non-degenerate, with a complete set of orthonormal eigenfunctions $\{|\phi_n\rangle\}$. Take the matrix element of both sides of the equation derived above between $\langle\phi_n|$ and $|\phi_n\rangle$. Insert a complete set of states $\sum_k |\phi_k\rangle\langle\phi_k| = I$ appropriately, to get the identity

$$\sum_k (E_k - E_n)\,|\langle\phi_k|\,x\,|\phi_n\rangle|^2 = \cdots$$

Note that the right-hand side is independent of the potential!

Solutions

1. True (**T**) or false (**F**):

(a) **T**
(b) **T**
(c) **F**
(d) **T**
(e) **F**
(f) **T**
(g) **T**
(h) **T**
(i) **F**
(j) **F**
(k) **F**
(l) **T**
(m) **T**
(n) **T**
(o) **F**
(p) **F**
(q) **T**
(r) **F**
(s) **F**
(t) **T**
(u) **T**
(v) **T**
(w) **T**
(x) **F**

2. Fill in the blanks:

(a) $x^n \quad \text{and} \quad (-1)^n \dfrac{d^n}{dx^n}$.

(b) $A = \dfrac{2}{r}\dfrac{\partial}{\partial r}$.

(c) $-\frac{3}{4} \quad \text{and} \quad \frac{1}{4}$.

(d) $|\langle \alpha \,|\, \beta \rangle|^2 = e^{-|\alpha - \beta|^2}$.

(e) $0 \quad \text{and} \quad 1$.

(f) $\overline{n}^2 + \overline{n}$.

(g) J_1^2 , J_2^2 , J^2 , J_z .

(h) $|\, j_1 \,,\, j_2 \,;\, j_1 + j_2 \,,\, j_1 + j_2 \,\rangle$ and $|\, j_1 \,,\, j_2 \,;\, j_1 + j_2 \,,\, -j_1 - j_2 \,\rangle$ respectively.

(i) $\langle\, j_1 \,,\, j_2 \,;\, j \,,\, m \,|\, j_1 \,,\, j_2 \,;\, j' \,,\, m' \,\rangle = \delta_{jj'}\, \delta_{mm'}$.

(j) $\dfrac{|\, \frac{1}{2} \,,\, \frac{1}{2} \,;\, \frac{1}{2} \,,\, -\frac{1}{2} \,\rangle - |\, \frac{1}{2} \,,\, \frac{1}{2} \,;\, -\frac{1}{2} \,,\, \frac{1}{2} \,\rangle}{\sqrt{2}}$, which is precisely $\dfrac{(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$.

(k) $a_{ij} = \sqrt{j}\ \delta_{i+1,j}$, where i and j run over the values $0, 1, 2, \ldots$ *ad inf.*

(l) $|\uparrow\rangle = \dfrac{|\rightarrow\rangle + |\leftarrow\rangle}{\sqrt{2}}$.

(m) $E_n = \hbar\omega\left(n + \frac{1}{2}\right) + \dfrac{3\lambda\hbar^2}{16m^2\omega^2}(2n^2 + 2n + 1)$.

(n) $\mathbf{j}(\mathbf{r}, t) = \dfrac{\hbar}{2mi}\,[\psi^* \nabla\psi - \psi\, \nabla\psi^*]$.

(o) $\mathbf{j}(\mathbf{r}, t) = \dfrac{\hbar k}{m}\,\dfrac{|A|^2}{r^2}\,\mathbf{e}_r$.

(p) $\big[\, x \,,\, [\, x \,,\, H \,]\,\big] = -\dfrac{\hbar^2}{m}$.

(q) $\displaystyle\sum_k (E_k - E_n)\,|\langle \phi_k |\, x \,|\phi_n\rangle|^2 = \frac{\hbar^2}{2m}$ (the Thomas-Reiche-Kuhn sum rule).