Mathematical background and revision

A.1 Vector spaces

Vectors and operators in finite spaces

Vectors in a **vector space** are members of a set for which addition and scalar multiplication both yield new members of the set. The familiar displacement and velocity vectors in real 3-D space are only some examples of vectors, and many more abstract instances occur in physics. In particular, the state of a quantum system is a vector in an infinite-dimensional vector space, and the possibility of *superposition*, which is one of the main ways in which classical and quantum descriptions of objects differ, follows. We denote vectors as $|\cdots\rangle$, eg $|v\rangle$, $|3\rangle$, $|\psi\rangle$, $|+\rangle$, $|\heartsuit\rangle$, where the text between the "|" and the "⟩" is just a name or label for the ket, which can take many forms. The **dimension** of the space is the size of the largest set of vectors which can be linearly independent, and such a set is a called a **basis**. Any vector in the space can be written as a sum over basis vectors

$$|v\rangle = \sum_{n=1}^{N} v_n |n\rangle$$

and the numbers v_n are called the **coefficients** or **components** of the vector in that basis. For a given basis, specifying the components specifies the vector.

Multiplying any vector by zero gives the null vector, which properly should be written $|0\rangle$ but is often written simply as 0. Indeed in QM, $|0\rangle$ may denote the ground state of a system, and in quantum field theory it may denote the vacuum.

We are usually concerned with spaces in which two vectors can be combined to give a complex number; this is the **inner product** which is written $\langle w|v\rangle = \langle v|w\rangle^*$. Note that if $|w\rangle = \alpha|a\rangle + \beta|b\rangle$, α and β being complex numbers, then $\langle w|v\rangle = \alpha^*\langle a|v\rangle + \beta^*\langle b|v\rangle$ This is called conjugate- or skew-linearity.

We may write vectors of a basis as $\{|v_1\rangle, |v_1\rangle \ldots |v_N\rangle\}$ or simply as $\{|1\rangle, |2\rangle \ldots |N\rangle\}$. It is very useful to work with **orthonormal** bases for which $\langle m|n\rangle = \delta_{mn}$.

When the vectors we are talking about are ordinary vectors in real 3-D space, we will tend not to use Dirac notation. Cartesian unit vectors forming an orthonormal basis in that space will be written $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. Here the inner product is the familiar scalar product.

Operators act on vectors to produce new vectors: $\hat{Q}|v\rangle = |w\rangle$. The **matrix element** of $\hat{Q}$ between two vectors is defined as $\langle u|\hat{Q}|v\rangle = \langle u|w\rangle$. The **identity operator** $\hat{I}$ leaves vectors

unchanged.

The object $\hat{A} = |u\rangle\langle v|$ is an operator, since it can act on a vector to give another (which will always be proportional to $|u\rangle$): $\hat{A}|w\rangle = (\langle v|w\rangle)|u\rangle$. If the vectors $\{|n\rangle\}$ form an orthonormal basis, then

$$\sum_{n=1}^{N} |n\rangle\langle n| = \hat{I} \qquad \text{since} \qquad \left(\sum_{n=1}^{N} |n\rangle\langle n|\right)|v\rangle = \sum_{n=1}^{N} |n\rangle\langle n|v\rangle = \sum_{n=1}^{N} v_n|n\rangle = |v\rangle.$$

This is called the **completeness relation**.

An operator is fully defined by what it does to the vectors of a basis, since then we can find what it does to any other vector. For each basis vector $|n\rangle$, $\hat{Q}|n\rangle$ is a new vector which can itself be expanded in the basis: $\hat{Q}|n\rangle = \sum_m^N Q_{mn}|m\rangle$. These N^2 numbers Q_{nm} fully define the operator, in the same way that the components of vector fully define it (always with respect to a given basis of course). With an orthonormal basis, we have

$$v_n = \langle n|v\rangle, \qquad Q_{mn} = \langle m|\hat{Q}|n\rangle \qquad \text{and} \qquad w_m = \sum_n^N Q_{mn}v_n.$$

The final equation is reminiscent of matrix multiplication. We can write the components of a vector as a vertical list (or column vector), and of an operator as a matrix, to give:

$$|v\rangle \longrightarrow \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} = \begin{pmatrix} \langle 1|v\rangle \\ \langle 2|v\rangle \\ \vdots \\ \langle N|v\rangle \end{pmatrix} \equiv \mathbf{v},$$

$$\langle v| \longrightarrow (v_1^*, u_2^*, \ldots v_N^*) = (\langle 1|v\rangle, \langle v|2\rangle, \ldots \langle v|N\rangle) \equiv \mathbf{v}^\dagger,$$

$$\hat{Q} \longrightarrow \begin{pmatrix} Q_{11} & Q_{12} & \ldots & Q_{1N} \\ Q_{21} & Q_{22} & \ldots & Q_{2N} \\ \vdots & \vdots & \vdots\vdots\vdots & \vdots \\ Q_{N1} & Q_{N2} & \ldots & Q_{NN} \end{pmatrix} = \begin{pmatrix} \langle 1|\hat{Q}|1\rangle & \langle 1|\hat{Q}|2\rangle & \ldots & \langle 1|\hat{Q}|N\rangle \\ \langle 2|\hat{Q}|1\rangle & \langle 2|\hat{Q}|2\rangle & \ldots & \langle 2|\hat{Q}|N\rangle \\ \vdots & \vdots & \vdots\vdots\vdots & \vdots \\ \langle N|\hat{Q}|1\rangle & \langle N|\hat{Q}|2\rangle & \ldots & \langle N|\hat{Q}|N\rangle \end{pmatrix} \equiv \mathbf{Q}.$$

The Q_{mn} are called the matrix elements of $\hat{Q}$ in this basis. So

$$\langle u|\hat{Q}|v\rangle = (u_1^*, u_2^*, \ldots u_N^*) \begin{pmatrix} Q_{11} & Q_{12} & \ldots & Q_{1N} \\ Q_{21} & Q_{22} & \ldots & Q_{2N} \\ \vdots & \vdots & \vdots\vdots\vdots & \vdots \\ Q_{N1} & Q_{N2} & \ldots & Q_{NN} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} = \mathbf{u}^\dagger\mathbf{Q}\mathbf{v}$$

The symbol $\underset{name}{\longrightarrow}$ means "**is represented by**", with *name* being a name or label for the basis, which will be omitted if the basis is obvious. In different bases, the components and matrix elements will be different. The corresponding column vectors and matrices are *different representations of the same vector/operator*. (Note though that $\langle u|\hat{Q}|v\rangle$ is a just number and independent of the representation.)

Note that in their own basis, the basis vectors themselves have extremely simple representations: in a 3-D space, if we use the symbol $\underset{\{1,2,3\}}{\longrightarrow}$ to mean "is represented in the $\{|1\rangle, |2\rangle, |3\rangle\}$ basis

by", then

$$|1\rangle \underset{\{1,2,3\}}{\longrightarrow} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |2\rangle \underset{\{1,2,3\}}{\longrightarrow} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |3\rangle \underset{\{1,2,3\}}{\longrightarrow} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

If we choose a new orthonormal basis $\{|n'\rangle\}$, vectors and operators will have new coefficients. With $v_n = \langle n|v\rangle$, $v'_n = \langle n'|v\rangle$, $Q_{mn} = \langle m|\hat{Q}|n\rangle$ and $Q'_{mn} = \langle m'|\hat{Q}|n'\rangle$, and where $\mathbf{S}$ is a unitary matrix (not an representing an operator) defined as $S_{mn} = \langle m|n'\rangle$, we have the following relations between the two representations:

$$v'_n = \sum_j S^*_{mn}\, v_m \Rightarrow \mathbf{v}' = \mathbf{S}^\dagger \mathbf{v}; \qquad Q'_{ij} = S^*_{ki} Q_{kl} S_{lj} \Rightarrow \mathbf{Q}' = \mathbf{S}^\dagger \mathbf{Q} \mathbf{S}.$$

For instance the vectors

$$|1'\rangle = \tfrac{1}{2}|1\rangle + \tfrac{i}{\sqrt{2}}|2\rangle - \tfrac{1}{2}|3\rangle, \quad |2'\rangle = \sqrt{\tfrac{1}{2}}(|1\rangle + |3\rangle), \quad |3'\rangle = \tfrac{1}{2}|1\rangle - \tfrac{i}{\sqrt{2}}|2\rangle - \tfrac{1}{2}|3\rangle$$

are orthonormal and so also form a basis. But in this new basis, the column vectors and matrices which represent states and operators will be different. For instance if $|v\rangle = |1\rangle - |3\rangle = |1'\rangle + |3'\rangle$ we write

$$|v\rangle \underset{\{1,2,3\}}{\longrightarrow} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \equiv \mathbf{v} \qquad |v\rangle \underset{\{1',2',3'\}}{\longrightarrow} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \equiv \mathbf{v}',$$

and

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \sqrt{\frac{1}{2}} & \frac{1}{2} \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ -\frac{1}{2} & \sqrt{\frac{1}{2}} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} v'_1 \\ v'_2 \\ v'_3 \end{pmatrix}.$$

The matrix is $\mathbf{S}$ as defined above. We observe that its columns are just the representations of the new states $\{|1'\rangle, |2'\rangle, |3'\rangle\}$ in the old basis $\{|1\rangle, |2\rangle, |3\rangle\}$: $S_{23} = \langle 2|3'\rangle$ etc.

The **adjoint** of an operator is defined by $\langle u|\hat{Q}|v\rangle = \langle v|\hat{Q}^\dagger|u\rangle^*$. A **unitary** operator satisfies $\hat{Q}^\dagger\hat{Q} = \hat{I}$.

A **Hermitian operator** is its own adjoint: $\langle u|\hat{Q}|v\rangle = \langle v|\hat{Q}|u\rangle^*$. In practice that means that $\hat{Q}$ can act backwards on $\langle u|$ or forward on $|v\rangle$, whichever is more convenient. In an orthonormal basis, $\hat{Q}$ will be represented by an matrix which equals its adjoint (transposed complex-conjugate): $Q_{mn} = Q^*_{nm}$.

Hermitian operators have real eigenvalues and orthogonal eigenvectors which span the space. (If eigenvalues are repeated, all linear combinations of the corresponding eigenvectors are also eigenvectors—they form a **degenerate subspace**—but an orthogonal subset can always be chosen.) Thus the normalised eigenvectors of Hermitian operators are often chosen as a basis, typically labelled by the eigenvalues: $|\lambda_n\rangle$. Two Hermitian operators which commute will have a common set of eigenvectors with might be labelled by both eigenvalues: $|\mu_m, \lambda_n\rangle$.

In its own eigenbasis, a Hermitian operator will be diagonal, with the eigenvalues as the diagonal elements. Hence the process of finding the eigenvalues and eigenvectors is often called **diagonalisation**. The unitary matrix $\mathbf{S}$ whose columns are the normalised eigenvectors can

be used to transform other vectors and operators to this basis.

Since we can add and multiply operators and multiply them by scalars, we can form power series of an operator and hence define more general functions via their power-series expansion. The most important **function of an operator** is the exponential:

$$\mathrm{e}^{\hat{Q}} \equiv \sum_{n=0}^{\infty} \frac{\hat{Q}^n}{n!}.$$

Since the corresponding power series for e^λ converges for all finite numbers, this is defined for all Hermitian operators, and its eigenvalues are e^{λ_i}. (In the eigenbasis of a Hermitian operator, any function of he operator is also represented by a diagonal matrix whose elements are the function of the eigenvalues.)

The exponential of a Hermitian operator is a unitary operator.

Functions as vectors

pth-order polynomials in the real variable x (with complex coefficients) form an $(p+1)$-D vector space. For $p = 3$, one examples of a base in this space would be $\{1, x, x^2, x^3\}$, and the representation of $|v\rangle = v_0 + v_1 x + v_2 x^2 + v_3 x^3$ in that basis is just the column vector $(v_0, v_1, v_2, v_3)^\top$. Another possible basis would be the first four Hermite polynomials

$$\{H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) = 4x^2 - 2, \quad H_3(x) = 8x^3 - 12x\}.$$

in which basis $|v\rangle \longrightarrow (v_0 + v_2/2, v_1/2 + 3v_3/4, v_2/4, v_3/8)^\top$.

More general sets of functions can also form vector spaces, but typically infinite-dimensional ones, with basis sets involving infinitely many functions. An example would be the set of all smooth functions $f(x)$ for which $\int_{-\infty}^{\infty} |f(x)|^2 \,\mathrm{d}x$ is finite. We take this as the definition of $\langle f|f\rangle$, with

$$\langle f|g\rangle = \int_{-\infty}^{\infty} f^*(x) g(x) \,\mathrm{d}x.$$

An example of an orthonormal basis for these functions is the set

$$\{|n\rangle = N_n H_n(x) \mathrm{e}^{-x^2/2}\} \quad \text{for } n = 0, 1, 2 \ldots$$

where N_n is a normalisation constant. Then any such function can be represented by an (infinitely long) list of numbers $|f\rangle \longrightarrow \big(\langle 0|f\rangle, \langle 1|f\rangle, \ldots\big)^\top$.

If we shift our perspective, we can consider the vectors in a infinite-dimensional space as primary, and the functions as just another representation—the **position-space representation**, in which $|f\rangle \underset{x}{\longrightarrow} f(x)$. With that viewpoint, the value $f(x_0)$ of the function at some value $x = x_0$ is like a component of the vector, and can be found by taking the inner product with a vector that picks out just that value, $|x_0\rangle$: $f(x_0) = \langle x_0|f\rangle$. If we don't want to specify a particular value, we have $f(x) = \langle x|f\rangle$ for the variable x.

With an eye on QM, we will often refer to vectors in a general vector space as **states**, which also helps to distinguish them from position and momentum vectors (of which more later).

Operators act on functions to turn one function into another; two simple examples are multiplication by x, and differentiation with respect to x. For their action on the abstract states, we use $\hat{x}$ and $\hat{D}$, and we need[1]

$$\langle x|\hat{x}|f\rangle = xf(x), \qquad \langle x|\hat{D}|f\rangle = \tfrac{\mathrm{d}f}{\mathrm{d}x}.$$

Since $\int f^* x g \,\mathrm{d}x = (\int g^* x f \,\mathrm{d}x)^*$, $\hat{x}$ is Hermitian. So we see that $|x\rangle$ is an eigenstate of $\hat{x}$:

$$\hat{x}|x_0\rangle = x_0|x_0\rangle \qquad \text{and} \qquad \hat{x}|x\rangle = x|x\rangle.$$

These position eigenstates satisfy (where x and x' are both values of the position variable)

$$\langle x'|x\rangle = \delta(x'-x), \qquad \int_{-\infty}^{\infty} |x\rangle\langle x| \,\mathrm{d}x = \hat{I}, \qquad \langle f|g\rangle = \langle f|\hat{I}|g\rangle = \int_{-\infty}^{\infty} f^*(x)g(x)\,\mathrm{d}x.$$

Also since $\int f^* \frac{\mathrm{d}g}{\mathrm{d}x}\,\mathrm{d}x = -(\int g^* \frac{\mathrm{d}f}{\mathrm{d}x}\,\mathrm{d}x)^*$, $\hat{D}$ is anti-hermitian, so $i\hat{D}$ is Hermitian. In QM we work with $\hat{p} = -i\hbar\hat{D}$, and we can see that $[\hat{x},\hat{p}] = i\hbar$. In the abstract vector space, this commutation relation defines $\hat{p}$. In position space, these operators are represented by[2]

$$\hat{x} \underset{x}{\longrightarrow} x, \qquad \hat{p} \underset{x}{\longrightarrow} -i\hbar\tfrac{\mathrm{d}}{\mathrm{d}x}.$$

We can define eigenstates of $\hat{p}$, $|p\rangle$, which have the following representation in position space:

$$|p\rangle \underset{x}{\longrightarrow} \langle x|p\rangle = \tfrac{1}{\sqrt{2\pi\hbar}}\,\mathrm{e}^{ipx/\hbar},$$

and which satisfy

$$\langle p'|p\rangle = \delta(p'-p), \qquad \int_{-\infty}^{\infty} |p\rangle\langle p|\,\mathrm{d}p, = \hat{I} \qquad \langle f|g\rangle = \langle f|\hat{I}|g\rangle = \int_{-\infty}^{\infty} \tilde{f}^*(p)\tilde{g}(p)\,\mathrm{d}p.$$

Up to factors of $\hbar$, $\langle p|f\rangle = \tilde{f}(p)$ is the Fourier transform of $f(x)$, and is an equally valid representation—in what we call **momentum space**—of the abstract state $|f\rangle$. The numerical equality of $\langle f|g\rangle$ calculated in the position and momentum representations is a reflection of Parseval's theorem.

We note that the states $|n\rangle$ defined above whose position-space representation is a Hermite polynomial times a Gaussian are actually eigenstates of $\hat{x}^2 - \hat{D}^2$, with eigenvalues $\lambda_n = 2n+1$. In this basis $\hat{x}$ and $\hat{p}$ are represented by infinite-dimensional matrices, and it can be shown that for both, only matrix elements where m and n differ by ± 1 are non-zero.

In the extension to functions of three coordinates x, y and z there are operators associated with each, $\hat{x}$, $\hat{y}$ and $\hat{z}$, which commute, and corresponding momentum operators $\hat{p}_x$, $\hat{p}_y$ and $\hat{p}_z$, which also commute. Between the two sets the only non-vanishing commutators are $[\hat{x},\hat{p}_x] = [\hat{y},\hat{p}_y] = [\hat{z},\hat{p}_z] = i\hbar$.

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[1] Shankar uses $\hat{X}$ for a dimensionless position variable, and $\hat{K} = -i\hat{D}$ as a dimensionless version of $\hat{p}$, but we stick with the QM notation.

[2] actually as these are operators, it is more accurate to give the matrix elements $\hat{x} \underset{x}{\longrightarrow} \langle x'|\hat{x}|x\rangle = x\delta(x'-x)$ and $\hat{p} \underset{x}{\longrightarrow} \langle x'|\hat{p}|x\rangle = -i\hbar\frac{\mathrm{d}\delta(x-x')}{\mathrm{d}x'}$, which then are integrated over x' in any expression, but as this has just the net effect of setting x' to x we never bother with this more correct version.

The position operator, $\hat{\mathbf{x}}$, is $\hat{x}\,\mathbf{e}_x + \hat{y}\,\mathbf{e}_y + \hat{z}\,\mathbf{e}_z$ in a particular Cartesian coordinate system[3], and similarly $\hat{\mathbf{p}}$. Boldface-and-hat now indicates a **vector operator**, i.e. a triplet of operators. The eigenstate of position is $|x, y, z\rangle \equiv |\mathbf{r}\rangle$:

$$\hat{\mathbf{x}}|\mathbf{r}\rangle = \big(\hat{x}\,\mathbf{e}_x + \hat{y}\,\mathbf{e}_y + \hat{z}\,\mathbf{e}_z\big)|\mathbf{r}\rangle = \big(x\,\mathbf{e}_x + y\,\mathbf{e}_y + z\,\mathbf{e}_z\big)|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle,$$
$$\hat{\mathbf{p}}|\mathbf{p}\rangle = \big(\hat{p}_x\,\mathbf{e}_x + \hat{p}_y\,\mathbf{e}_y + \hat{p}_z\,\mathbf{e}_z\big)|\mathbf{p}\rangle = \big(p_x\,\mathbf{e}_x + p_y\,\mathbf{e}_y + p_z\,\mathbf{e}_z\big)|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle.$$

In position space, $\hat{\mathbf{x}} \underset{\mathbf{r}}{\longrightarrow} \mathbf{r}$ and $\hat{\mathbf{p}} \underset{\mathbf{r}}{\longrightarrow} -i\hbar\nabla$. Momentum eigenstates are

$$|\mathbf{p}\rangle \underset{\mathbf{r}}{\longrightarrow} \langle\mathbf{r}|\mathbf{p}\rangle = \big(\tfrac{1}{2\pi}\big)^{3/2}\,\mathrm{e}^{i\mathbf{p}\cdot\mathbf{r}/\hbar},$$

which is a plane wave travelling in the direction of $\mathbf{p}$. Also

$$\langle f|g\rangle = \int_{-\infty}^{\infty} f^*(\mathbf{r})g(\mathbf{r})\,\mathrm{d}^3r, \qquad \langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}') = \delta(x-x')\delta(y-y')\delta(z-z').$$

Commutators

Let $\hat{A}$, $\hat{B}$ and $\hat{C}$ be arbitrary operators in some space. Then the following relations are very useful:

$$\begin{aligned}
\hat{A}\hat{B} &= \hat{B}\hat{A} + [\hat{A}, \hat{B}],\\
[\hat{A}, \hat{B}\hat{C}] &= [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}],\\
[\hat{A}\hat{B}, \hat{C}] &= [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}],\\
[\hat{A}, \hat{B}^n] &= n[\hat{A}, \hat{B}]\hat{B}^{n-1} \quad \text{provided } [\hat{A}, \hat{B}] \text{ commutes with } \hat{B}.\\
\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}} &= \mathrm{e}^{\hat{A}+\hat{B}+[\hat{A},\hat{B}]/2} \quad \text{provided } [\hat{A}, \hat{B}] \text{ commutes with } \hat{A} \text{ and } \hat{B}.
\end{aligned}$$

Let $Q(x)$ be a polynomial with derivative $R(x)$. Then

$$[\hat{p}_x, Q(\hat{x})] = -i\hbar R(\hat{x}) \qquad \Rightarrow\ [\hat{p}_x, Q(\hat{x})] \underset{x}{\longrightarrow} -i\hbar\tfrac{\mathrm{d}Q(x)}{\mathrm{d}x}.$$

Similarly if $V(\mathbf{r})$ is a function of position in 3-D,

$$[\hat{\mathbf{p}}, V(\hat{\mathbf{x}})] \underset{\mathbf{r}}{\longrightarrow} -i\hbar\,\nabla V(\mathbf{r}).$$

[3] we do not use $\hat{\mathbf{r}}$ since that is reserved for the unit vector $\mathbf{r}/r$!

A.2 Series Solution of Hermite's equation and the Harmonic Oscillator

Shankar 7.3
Griffiths 2.3.2

We consider a particle moving in a 1D quadatic potential $V(x) = \frac{1}{2}m\omega^2 x^2$, like a mass on a spring. The Hamiltonian operator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{A.1}$$

We will work in rescaled dimensionless coordinates, defining the length scale $x_0 = \sqrt{\hbar/m\omega}$, so $\hat{x} \to x_0 y$ and $\hat{p} \to (-i\hbar/x_0)\mathrm{d}/\mathrm{d}y$. The energy scale is $\frac{1}{2}m\omega^2 x_0^2 = \frac{1}{2}\hbar\omega$. We are looking for wave functions $\phi(y)$, of energy $E = \frac{1}{2}\hbar\omega\mathcal{E}$, which satisfy

$$-\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} + y^2\phi = \mathcal{E}\phi. \tag{A.2}$$

If we write $\phi(y) \equiv f(y)\mathrm{e}^{-y^2/2}$, this can be rewritten as

$$\frac{\mathrm{d}^2 f}{\mathrm{d}y^2} - 2y\frac{\mathrm{d}f}{\mathrm{d}y} + (\mathcal{E}-1)f = 0. \tag{A.3}$$

This is Hermite's differential equation. If we look for a series solution of the form $f(y) = \sum_{j=0}^{\infty} c_j y^n$, we get

$$\sum_{j=2}^{\infty} j(j-1)c_j y^{j-2} - 2\sum_{j=1}^{\infty} j c_j y^j + (\mathcal{E}-1)\sum_{j=0}^{\infty} c_n y^j = 0$$

$$\Rightarrow \qquad \sum_{j=0}^{\infty}\Big((j+1)(j+2)c_{j+2} + (\mathcal{E}-1-2j)c_j\Big)y^j = 0 \tag{A.4}$$

where we have changed the summation index in the first sum before relabelling it j. The only way a polynomial can vanish for all y is if all the coefficients vanish, so we have a *recurrence relation*:

$$(j+1)(j+2)c_{j+2} + (\mathcal{E}-1-2j)c_j = 0. \tag{A.5}$$

Given c_0 and c_1, we can construct all other coefficients from this equation, for any $\mathcal{E}$. We can obtain two independent solution, as expected for a second order differential equation: even solutions with $c_1 = 0$ and odd ones with $c_0 = 0$.

However, we need the wave function to be *normalisable* (square integrable), which means that it tends to 0 as $x \to \pm\infty$. In general an infinite polynomial times a Gaussian will not satisfy this, and these solutions are not physically acceptable. If we look again at equation (A.5), though, we see that if $\mathcal{E} = 1 + 2n$ for some integer $n \geq 0$, then c_{n+2}, c_{n+4}, $c_{n+6}\ldots$ are all zero. Thus for $\mathcal{E} = 1, 5, 9\ldots$ we have finite even polynomials, and for $\mathcal{E} = 3, 7, 11\ldots$ we have finite odd polynomials. These are called the Hermite polynomials.

Rewriting (A.5) with $\mathcal{E} = 1 + 2n$ as

$$c_{j+2} = \frac{2(j-n)}{(j+1)(j+2)}c_j, \tag{A.6}$$

we have for instance, for $n = 5$,

$$c_3 = 2(1-5)c_1/(2.3) = -4c_1/3 \qquad c_5 = 2(3-5)c_3/(4.5) = -c_3/5 = 4c_1/15, \qquad c_7 = c_9 = \ldots = 0, \tag{A.7}$$

and $H_5(y) = c_1(4y^5 - 20y^3 + 15y)/15$. The conventional normalisation uses 2^n for the coefficient of the highest power of y, which would require $c_1 = 120$, and $H_5(y) = 32y^5 - 160y^3 + 120y$. The first four are:

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

The corresponding solutions of the original Hamiltonian, returning to unscaled coordinates, are

$$\phi_n(x) = (2^n n!)^{-1/2} H_n(\tfrac{x}{x_0}) \times (\pi x_0^2)^{-1/4} \exp\bigl(-x^2/(2x_0^2)\bigr);$$

with energies $E_n = (n + \frac{1}{2})\hbar\omega$.

Just as in the square well, the restriction to solutions which satisfy the boundary conditions has resulted in quantised energy levels.

The wave functions and probablility densities are illustrated below.

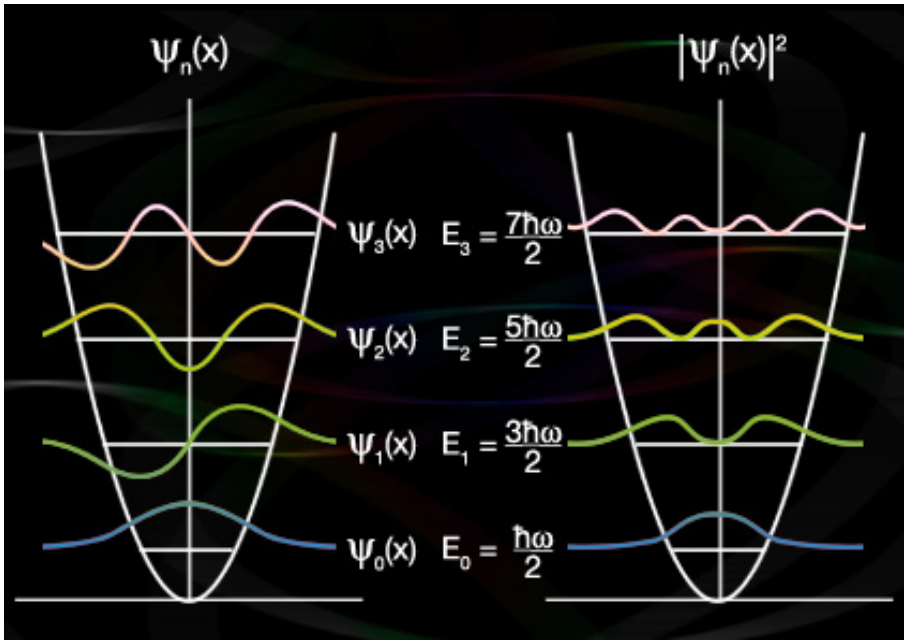


Figure A.1: Energy levels and wave functions of the Harmonic oscillator, from Florida State University Physics wiki:
http://wiki.physics.fsu.edu/wiki/index.php/Harmonic_Oscillator_Spectrum_and_Eigenstates

A.3 Angular Momentum in Quantum Mechanics

The following section was prepared in another contex and so does not use Dirac notation; I would use $|\uparrow\rangle$ etc for spi states.

Orbital angular momentum

We start with the classical definition of orbital angular momentum. In quantum mechanics the position and momentum vectors become operators, so

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \Rightarrow \hat{L}_z = -i\hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right) = -i\hbar \frac{\partial}{\partial \phi} \quad \text{etc}$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z \quad \text{etc}; \qquad [\hat{\mathbf{L}}^2, \hat{L}_i] = 0;$$

The commutation relations imply that we can only simultaneously know $\mathbf{L}^2$ and one component, taken conventionally to be L_z. The common eigenfunctions of $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ are the spherical harmonics, $Y_l^m(\theta, \phi)$:

$$\hat{\mathbf{L}}^2 Y_l^m(\theta,\phi) = \hbar^2\, l(l+1)\, Y_l^m(\theta,\phi) \qquad \hat{L}_z Y_l^m(\theta,\phi) = \hbar m\, Y_l^m(\theta,\phi)$$

From requirements that the wave function must be finite everywhere, and single-valued under $\phi \to \phi + 2\pi$, it emerges that l and m are integers and must satisfy

$$l = 0, 1, 2 \ldots, \qquad\qquad m = -l, -l+1, \ldots l.$$

These have definite parity of $(-1)^l$, since under $\mathbf{r} \to -\mathbf{r}$,

$$Y_l^m(\theta,\phi) \to Y_l^m(\pi - \theta, \phi + \pi) = (-1)^l Y_l^m(\theta,\phi).$$

See the end of these notes for some explicit forms of spherical harmonics.

Intrinsic and total angular momentum

Orbital angular momentum is not the only source of angular momentum, particles may have *intrinsic angular momentum or spin*. The corresponding operator is $\hat{\mathbf{S}}$. The eigenvalues of $\hat{\mathbf{S}}^2$ have the same form as in the orbital case, $\hbar^2 s(s+1)$ but now s can be integer or half integer; similarly the eigenvalues of $\hat{S}_z$ are $\hbar m_s$, with

$$s = 0, \tfrac{1}{2}, 1, \tfrac{3}{2} \ldots, \qquad\qquad m_s = -s, -s+1, \ldots s.$$

$s = \frac{1}{2}$ for an electron, $s = 1$ for a photon or W boson. This means that the magnitude of the spin vector of an electron is $(\sqrt{3}/2)\hbar$, but we always just say "spin-$\frac{1}{2}$".

If a particle has both orbital and spin angular momentum, we talk about its *total angular momentum*, with operator

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}.$$

As with spin, the eigenvalues of $\hat{\mathbf{J}}^2$ are $\hbar^2 j(j+1)$

$$j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2} \ldots, \qquad\qquad m_j = -j, -j+1, \ldots j.$$

Systems composed of more than one particle (hadrons, nuclei, atoms) will have many contributions to their total angular momentum. It is sometimes useful to add up all the spins to give a total spin, and now, confusingly, we denote the quantum numbers by S and M_S, so it is really important to distinguish operators and the corresponding quantum numbers. Then

$$\hat{\mathbf{S}}^{\rm tot} = \hat{\mathbf{S}}^{(1)} + \hat{\mathbf{S}}^{(2)} + \ldots,$$

where the superscripts (1), (2) refer to the individual particles.

Similarly we use $\hat{\mathbf{L}}^{\rm tot}$ with quantum numbers L and M_L, and $\hat{\mathbf{J}}^{\rm tot}$ with quantum numbers J and M_J. When talking about angular momentum generally, we often use $\hat{\mathbf{J}}$ to refer to *a*ny angular momentum, whether single or multiple particle, pure spin, pure orbital or a combination.

The following rules are obeyed by *a*ny angular momentum (eg $\hat{\mathbf{J}}$ can be replaced by $\hat{\mathbf{L}}$ or $\hat{\mathbf{S}}$, for a single particle of composite system):

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z \quad \text{etc;} \qquad [\hat{\mathbf{J}}^2, \hat{J}_i] = 0;$$

It follows that the eigenvalues of $(\hat{\mathbf{L}}^{\rm tot})^2$, $(\hat{\mathbf{S}}^{\rm tot})^2$ and $(\hat{\mathbf{J}}^{\rm tot})^2$ have exactly the same form, with the same restrictions on the quantum numbers, as those for a single particle. So for instance the eigenstates of $(\hat{\mathbf{S}}^{\rm tot})^2$ are $\hbar^2 S(S+1)$, and of $\hat{S}_z^{\rm tot}$ are $\hbar M_s$, and

$$L = 0, 1, 2 \ldots, \qquad S = 0, \tfrac{1}{2}, 1, \tfrac{3}{2} \ldots, \qquad J = 0, \tfrac{1}{2}, 1, \tfrac{3}{2} \ldots,$$

$$M_L = -L, -L+1, \ldots L, \qquad M_S = -S, -S+1, \ldots S, \qquad M_J = -J, -J+1, \ldots J.$$

Addition of angular momentum

The rules for the addition of angular momentum are as follows: we start with adding orbital angular momentum and spin for a composite system with quantum numbers L and S. Angular momentum is a vector, and so the total can be smaller as well as greater that the parts; however the z-components just add. The allowed values of the total angular momentum quantum numbers are

$$J = |L-S|, |L-S|+1, \ldots, L+S, \qquad M_J = M_L + M_S.$$

However since $\hat{L}_z$ and $\hat{S}_z$ do not commute with $\hat{\mathbf{J}}^2$, we cannot know J, M_L and M_S simultaneously. For a single-particle system, replace J, L, and S with j, l, and s.

More generally, for the addition of any two angular momenta with quantum numbers J_1, M_1 and J_2, M_2, the rules are

$$J = |J_1 - J_2|, |J_1 - J_2| + 1, \ldots, J_1 + J_2, \qquad M_J = M_1 + M_2$$

and again we cannot know J, M_1 and M_2 simultaneously.

Confusingly, when referring to a composite particle (eg a hadron or nucleus), the total angular momentum is often called its "spin" but given the quantum number J. Sometimes this usage even extends to elementary particles. For the electron and proton, s is more common though.

For the case of a spin-$\frac{1}{2}$ particle, the eigenvalues of $\hat{S}_z$ are $\pm\frac{1}{2}\hbar$, and here we will just denote these states by $\uparrow$ and $\downarrow$ (α_z and β_z are also often used); hence

$$\hat{\mathbf{S}}^2\uparrow = \frac{3}{4}\hbar^2\uparrow \qquad \hat{\mathbf{S}}^2\downarrow = \frac{3}{4}\hbar^2\downarrow$$
$$\hat{S}_z\uparrow = \tfrac{1}{2}\hbar\uparrow \qquad \hat{S}_z\downarrow = -\tfrac{1}{2}\hbar\downarrow$$

For two such particles there are four states $\uparrow\uparrow$, $\downarrow\downarrow$, $\uparrow\downarrow$ and $\downarrow\uparrow$. The first two states have $M_S = 1$ and -1 respectively, and we can show, using $\hat{\mathbf{S}}^{\rm tot} = \hat{\mathbf{S}}^{(1)} + \hat{\mathbf{S}}^{(2)}$, that they are also eigenstates of $(\hat{\mathbf{S}}^{\rm tot})^2$ with $S = 1$. However the second two, though they have $M_S = 0$, are not eigenstates of $(\hat{\mathbf{S}}^{\rm tot})^2$. To make those, we need linear combinations, tabulated below:

	$S = 1$	$S = 0$
$M = 1$	$\uparrow\uparrow$	
$M = 0$	$\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$	$\frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$
$M = -1$	$\downarrow\downarrow$	

The $S = 1$ states are symmetric under exchange of particles; the $S = 0$ states are antisymmetric. For a system of N spin-$\frac{1}{2}$ particles, S will be integer if N is even and half-integer if N is odd.

Bosons and Fermions

Particles with half-integer spin (electrons, baryons) are called fermions, those with integer spin, including $J = 0$, (mesons, photons, Higgs) are called bosons. The "Pauli exclusion principle" applies to fermions, but it is a special case of the "spin-statistics theorem" which says that the overall quantum state of a system of identical fermions must be antisymmetric under exchange of any pair, while that of a system of identical bosons must be symmetric. There may be several components to the state (spatial wave function, spin state...).

Examples of the consequences of the spin-statistics theorem are:

- If two electrons in an atom are in the same orbital (thus their spatial wave function is symmetric under exchange of the two), they must be in an $S = 0$ state.
- Thus the ground state of helium has $S = 0$, but the excited states can have $S = 0$ (parahelium) or $S = 1$ (orthohelium).
- Two π^0 mesons must have even relative orbital angular momentum L (they are spinless, so this is the only contribution to their wave function).
- Two ρ^0 mesons (spin-1 particles) can have odd or even relative orbital angular momentum L, but their spin state must have the same symmetry as their spatial state. (In this case, $S = 2$ and 0 are even, $S = 1$ is odd.)

Note that in the last two, in the centre-of-momentum frame the spatial state only depends on the relative coordinate $\mathbf{r}$. So interchanging the particles is equivalent to $\mathbf{r} \to -\mathbf{r}$, ie the parity operation.

Spherical Harmonics

In spherical polar coordinates the orbital angular momentum operators are

$$\begin{aligned}
\hat{L}_x &= \tfrac{1}{2}(\hat{L}_+ + \hat{L}_-) \quad \text{and} \quad \hat{L}_y = \tfrac{1}{2i}(\hat{L}_+ - \hat{L}_-), \quad \text{where} \\
\hat{L}_+ &= \hbar \mathrm{e}^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right), \qquad \hat{L}_- = \hat{L}_+^\dagger = \hbar \mathrm{e}^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right); \\
\hat{L}_z &= -i\hbar\frac{\partial}{\partial\phi}, \qquad \hat{\mathbf{L}}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right). \\
\nabla^2\psi &= \frac{1}{r}\frac{\partial^2}{\partial r^2}r\psi - \frac{1}{\hbar^2 r^2}\hat{\mathbf{L}}^2\psi;
\end{aligned}$$

The spherical harmonics, $Y_l^m(\theta,\phi)$ are eigenfunctions of $\hat{\mathbf{L}}^2$ and $\hat{L}_z$; the first few are as follows

$$\begin{aligned}
Y_0^0(\theta,\phi) &= \sqrt{\frac{1}{4\pi}} & Y_1^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{3}{8\pi}}\,\sin\theta\,\mathrm{e}^{\pm i\phi} \\
Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\,\cos\theta & Y_2^{\pm2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\,\mathrm{e}^{\pm 2i\phi} \\
Y_2^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}\,\sin\theta\,\cos\theta\,\mathrm{e}^{\pm i\phi} & Y_2^0(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta - 1)
\end{aligned}$$

A.4 Hydrogen wave functions

The solutions of the Schrödinger equation for the Coulomb potential $V(r) = -\hbar c\alpha/r$ have energy $E_n = -\frac{1}{n^2}E_{\rm Ry}$, where $E_{\rm Ry} = \frac{1}{2}\alpha^2 mc^2 = 13.6$ eV (with m the reduced mass of the electron-proton system). (Recall $\alpha = e^2/(4\pi\epsilon_0\hbar c) \approx 1/137$.) The spatial wavefunctions are $\psi_{nlm}(\mathbf{r}) = R_{n,l}(r)Y_l^m(\theta,\phi)$.

The radial wavefunctions are as follows, where $a_0 = \hbar c/(mc^2\alpha)$:

$$
\begin{aligned}
R_{1,0}(r) &= \frac{2}{a_0^{3/2}}\,\exp\left(-\frac{r}{a_0}\right),\\
R_{2,0}(r) &= \frac{2}{(2\,a_0)^{3/2}}\left(1-\frac{r}{2\,a_0}\right)\exp\left(-\frac{r}{2\,a_0}\right),\\
R_{2,1}(r) &= \frac{1}{\sqrt{3}\,(2\,a_0)^{3/2}}\,\frac{r}{a_0}\,\exp\left(-\frac{r}{2\,a_0}\right),\\
R_{3,0}(r) &= \frac{2}{(3\,a_0)^{3/2}}\left(1-\frac{2\,r}{3\,a_0}+\frac{2\,r^2}{27\,a_0^2}\right)\exp\left(-\frac{r}{3\,a_0}\right),\\
R_{3,1}(r) &= \frac{4\,\sqrt{2}}{9\,(3\,a_0)^{3/2}}\,\frac{r}{a_0}\left(1-\frac{r}{6\,a_0}\right)\exp\left(-\frac{r}{3\,a_0}\right),\\
R_{3,2}(r) &= \frac{2\,\sqrt{2}}{27\,\sqrt{5}\,(3\,a_0)^{3/2}}\left(\frac{r}{a_0}\right)^2\exp\left(-\frac{r}{3\,a_0}\right).
\end{aligned}
$$

They are normalised, so $\int_0^\infty (R_{n,l}(r))^2 r^2 {\rm d}r = 1$. Radial wavefuntions of the same l but different n are orthogonal (the spherical harmonics take care of orthogonality for different ls).

The following radial integrals can be proved:

$$
\begin{aligned}
\langle r^2\rangle &= \frac{a_0^2\,n^2}{2}\left(5\,n^2+1-3l\,(l+1)\right),\\
\langle r\rangle &= \frac{a_0}{2}\left(3n^2-l\,(l+1)\right),\\
\left\langle\frac{1}{r}\right\rangle &= \frac{1}{n^2 a_0},\\
\left\langle\frac{1}{r^2}\right\rangle &= \frac{1}{(l+1/2)\,n^3\,a_0^2},\\
\left\langle\frac{1}{r^3}\right\rangle &= \frac{1}{l\,(l+1/2)\,(l+1)\,n^3\,a_0^3}.
\end{aligned}
$$

For hydrogen-like atoms (single-electron ions with nuclear charge $|e|\,Z$) the results are obtained by substituting $\alpha \to Z\alpha$ (and so $a_0 \to a_0/Z$).

A.5 Properties of δ-functions

The δ-function is defined by its behaviour in integrals:

$$\int_a^b \delta(x-x_0)\mathrm{d}x = 1; \qquad \int_a^b f(x)\delta(x-x_0)\,\mathrm{d}x = f(x_0)$$

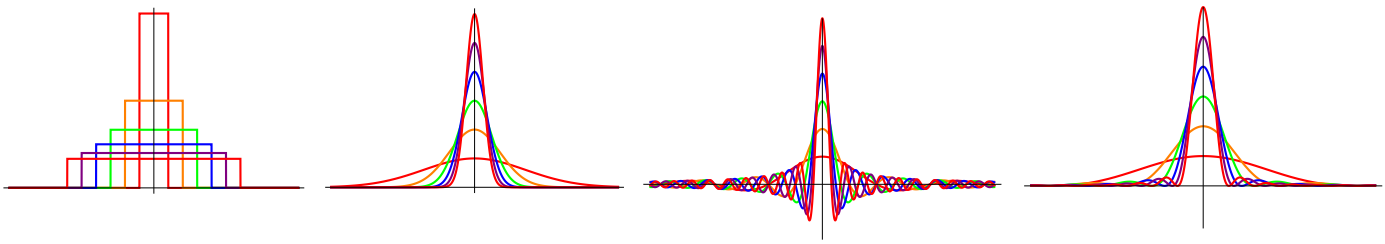
where the limits a and b satisfy $a < x_0 < b$; the integration simply has to span the point on which the δ-function is centred. The second property is called the **sifting property** because it picks out the value of f at $x = x_0$.

The following equivalences may also be proved by changing variables in the corresponding integral (an appropriate integration range is assumed for compactness of notation):

$$\begin{aligned} \delta(ax-b) &= \tfrac{1}{|a|}\delta(x-\tfrac{b}{a}) \qquad \text{since} \quad \int f(x)\delta(ax-b)\,\mathrm{d}x = \tfrac{1}{a}f(\tfrac{b}{a}) \\ \delta(g(x)) &= \sum_i \frac{\delta(x-x_i)}{|g'(x_i)|} \qquad \text{where the } x_i \text{ are the (simple) real roots of } g(x). \end{aligned}$$

Note that the dimensions of a δ-function are the inverse of those of its argument, as should be obvious from the first equation.

Though the δ-function is not well defined as a function (technically it is a distribution rather than a function), it can be considered as the limit of many well-defined functions. For instance the "top-hat" function which vanishes outside a range a and has height $1/a$ tends to a δ-function as $a \to \infty$. Similarly a Gaussian with width and height inversely proportial tends to a δ-function as the width tends to zero. These are shown in the first two frames below.

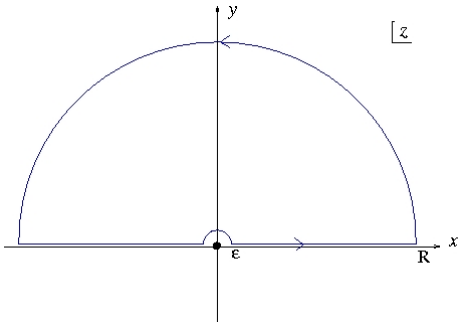


Two less obvious functions which tend to a δ-function, shown in the next two frames, are the following:

$$\begin{aligned} &\tfrac{1}{2\pi}\int_{-L}^{L} \mathrm{e}^{i(k-k')x}\,\mathrm{d}x = \tfrac{L}{\pi}\,\mathrm{sinc}\big((k-k')L\big) \overset{L\to\infty}{\longrightarrow} \delta(k-k') \\ &\tfrac{L}{\pi}\,\mathrm{sinc}^2\big((k-k')L\big) \overset{L\to\infty}{\longrightarrow} \delta(k-k') \end{aligned}$$

The first of these does not actually vanish away from the peak, but it oscillates so rapidly that there will be no contribution to any integral over k' except from the point $k' = k$. This is the integral which gives the orthogonality of two plane waves with different wavelengths: $\langle k|k'\rangle = \delta(k-k')$. It also ensures that the inverse Fourier transform of a Fourier transform recovers the original function.

That the normalisation (for integration over k) is correct follows from the following two integrals: $\int_{-\infty}^{\infty}\mathrm{sinc}(t)\mathrm{d}t = \pi$ and $\int_{-\infty}^{\infty}\mathrm{sinc}^2(t)\mathrm{d}t = \pi$. The second of these follows from the first via integration by parts. The integral $\int_{-\infty}^{\infty}\mathrm{sinc}(t)\mathrm{d}t = \mathrm{Im}\,I$ where $I = \int_{-\infty}^{\infty}\big(\mathrm{e}^{it}/t\big)\mathrm{d}t$ may be done via the contour integral below:



As no poles are included by the contour, the full contour integral is zero. By Jordan's lemma the integral round the outer circle tends to zero (as $R \to \infty$, e^{iz} decays exponentially in the upper half plane). So the integral along the real axis is equal and opposite to the integral over the inner circle, namely $-\pi i$ times the residue at $x = 0$, so $I = i\pi$. So the imaginary part, the integral of $\mathrm{sinc}(x)$, is π.

A.6 Gaussian integrals

The following integrals will be useful:

$$\int_{-\infty}^{\infty} \mathrm{e}^{-\alpha x^2} \mathrm{d}x = \sqrt{\frac{\pi}{\alpha}} \qquad \text{and} \qquad \int_{-\infty}^{\infty} x^{2n} \mathrm{e}^{-\alpha x^2} \mathrm{d}x = (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}\alpha^n} \left(\sqrt{\frac{\pi}{\alpha}} \right)$$

These work even for complex α, so long as $\mathrm{Re}\,[\alpha] \geq 0$

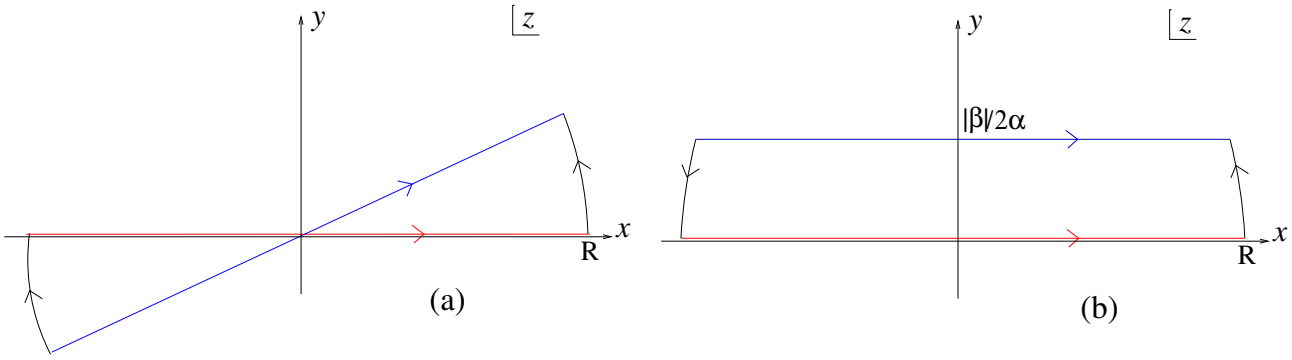
Often we are faced with a somewhat more complicated integral, which can be cast in Gaussian form by "completing the square" in the exponent and then shifting integration variable $x \to x - \beta/(2\alpha)$:

$$\int_{-\infty}^{\infty} \mathrm{e}^{-\alpha x^2 - \beta x} \mathrm{d}x = \mathrm{e}^{\beta^2/(4\alpha)} \int_{-\infty}^{\infty} \mathrm{e}^{-\alpha(x+\beta/(2\alpha))^2} \mathrm{d}x = \sqrt{\frac{\pi}{\alpha}} \mathrm{e}^{\beta^2/(4\alpha)}$$

This works even if β is imaginary.

The two contours below illustrate the two results for complex parameters α or β. For the first, in (a), we rewrite αx^2 as $|\alpha| z^2$ where $z = x \exp(i\mathrm{Arg}\,[\alpha]/2)$, so the integral we want is along the blue line, with $R \to \infty$. Since there are no poles, by Cauchy's theorem the integral along the blue contour must equal the sum of those along the red and black countours. As $R \to \infty$ the red one gives the known real integral. Since $\mathrm{e}^{-|\alpha| z^2}$ tends to zero faster than $1/R$ as $R \to \infty$ providing $|x| > |y|$, the contribution from the black paths is zero as $R \to \infty$. Hence the red and blue integrals are the same, provided $\mathrm{Arg}\,[\alpha] \leq \pi/2$.

For the second, in (b), the blue contour is the desired integral one after the variable change (for β imaginary). Again the red and black paths together must equal the blue and again the contribution from the black paths is zero. Hence the two integrals must be the same.

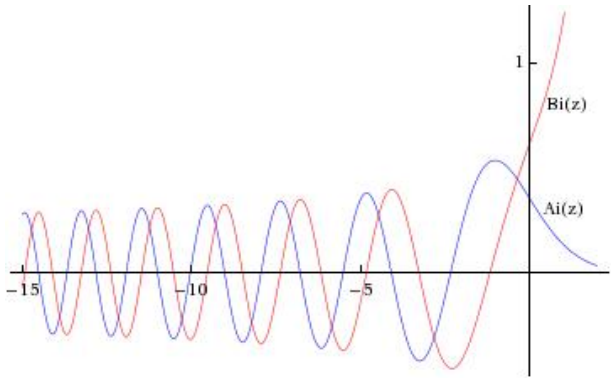


A.7 Airy functions

Airy functions are the solutions of the differential equation:

$$\frac{\mathrm{d}^2 f}{\mathrm{d}z^2} - zf = 0$$

There are two solutions, $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$; the first tends to zero as $z \to \infty$, while the second blows up. Both are oscillatory for $z < 0$. The Mathematica functions for obtaining them are



`AiryAi[z]` and `AiryBi[z]`.

The asymptotic forms of the Airy functions are:

$$\mathrm{Ai}(z) \overset{z\to\infty}{\longrightarrow} \frac{\mathrm{e}^{-\frac{2}{3}z^{3/2}}}{2\sqrt{\pi}z^{1/4}} \qquad \text{and} \qquad \mathrm{Ai}(z) \overset{z\to-\infty}{\longrightarrow} \frac{\cos\left(\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}\right)}{\sqrt{\pi}|z|^{1/4}}$$

$$\mathrm{Bi}(z) \overset{z\to\infty}{\longrightarrow} \frac{\mathrm{e}^{\frac{2}{3}z^{3/2}}}{\sqrt{\pi}z^{1/4}} \qquad \text{and} \qquad \mathrm{Bi}(z) \overset{z\to-\infty}{\longrightarrow} \frac{\cos\left(\frac{2}{3}|z|^{3/2} + \frac{\pi}{4}\right)}{\sqrt{\pi}|z|^{1/4}}$$

The Schrödinger equation for a linear potential $V(x) = \beta x$ in one dimension can be cast in the following form

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \beta x\psi - E\psi = 0$$

Defining $z = x/x_0$, with $x_0 = (\hbar^2/(2m\beta))^{1/3}$, and $E = (\hbar^2\beta^2/(2m))^{1/3}\mu$, and with $y(z) \equiv \psi(x)$, this can be written

$$\frac{\mathrm{d}^2 y}{\mathrm{d}z^2} - zy + \mu y = 0.$$

The solution is

$$y(z) = C\,\mathrm{Ai}(z-\mu) + D\,\mathrm{Bi}(z-\mu) \qquad \text{or} \qquad \psi(x) = C\,\mathrm{Ai}\big((\beta x - E)/(\beta x_0)\big) + D\,\mathrm{Bi}\big((\beta x - E)/(\beta x_0)\big)$$

where $D = 0$ if the solution has to extend to $x = \infty$. The point $z = \mu$, $x = E/\beta$ is the point at which $E = V$ and the solution changes from oscillatory to decaying / growing.

The equation for a potential with a negative slope is given by substituting $z \to -z$ in the defining equation. Hence the general solution is $\psi(x) = C\,\mathrm{Ai}(-x/x_0 - \mu) + D\,\mathrm{Bi}(-x/x_0 - \mu)$, with $D = 0$ if the solution has to extend to $x = -\infty$.

The first few zeros of the Airy functions are given in Wolfram MathWorld.

A.8 Units in EM

There are several systems of units in electromagnetism. We are familiar with SI units, but Gaussian units are still very common and are used, for instance, in Shankar.

In SI units the force between two currents is used to define the unit of current, and hence the unit of charge. (Currents are much easier to calibrate and manipulate in the lab than charges.) The constant μ_0 is *defined* as $4\pi \times 10^{-7}\ \mathrm{N\,A^{-2}}$, with the magnitude chosen so that the Ampère is a "sensible" sort of size. Then Coulomb's law reads

$$\mathbf{F} = \frac{q_1 q_2}{4\pi\epsilon_0 \left|\mathbf{r}_1 - \mathbf{r}_2\right|^2}$$

and ϵ_0 has to be obtained from experiment. (Or, these days, as the speed of light is now has a defined value, ϵ_0 is obtained from $1/(\mu_0 c^2)$.)

However one could in principle equally decide to use Coulomb's law to define charge. This is what is done in Gaussian units, where by definition

$$\mathbf{F} = \frac{q_1 q_2}{\left|\mathbf{r}_1 - \mathbf{r}_2\right|^2}$$

Then there is no separate unit of charge; charges are measured in $\mathrm{N^{1/2}\,m}$ (or the non-SI equivalent): $e = 4.803 \times 10^{-10}\ \mathrm{g^{1/2}\,cm^{3/2}\ s^{-1}}$. (You should never need that!) In these units, $\mu_0 = 4\pi/c^2$. Electric and magnetic fields are also measured in different units.

The following translation table can be used:

Gauss	e	$\mathbf{E}$	$\mathbf{B}$
SI	$e/\sqrt{4\pi\epsilon_0}$	$\sqrt{4\pi\epsilon_0}\,\mathbf{E}$	$\sqrt{4\pi/\mu_0}\,\mathbf{B}$

Note that $e\mathbf{E}$ is the same in both systems of units, but $e\mathbf{B}$ in SI units is replaced by $e\mathbf{B}/c$ in Gaussian units. Thus the Bohr magneton μ_B is $e\hbar/2m$ in SI units, but $e\hbar/2mc$ in Gaussian units, and $\mu_B\mathbf{B}$ has dimesions of energy in both systems.

The fine-structure constant α is a dimensionless combination of fundamental units, and as such takes on the same value ($\approx 1/137$) in all systems. In SI it is defined as $\alpha = e^2/(4\pi\epsilon_0\,\hbar c)$, in Gaussian units as $\alpha = e^2/(\,\hbar c)$. In all systems, therefore, Coulomb's law between two particles of charge $z_1 e$ and $z_2 e$ can be written

$$\mathbf{F} = \frac{z_1 z_2\ \hbar c \alpha}{\left|\mathbf{r}_1 - \mathbf{r}_2\right|^2}$$

and this is the form I prefer.