Appendix A
Vector and Matrix Analysis

A.1 Scalar Product

Consider two complex, n-dimensional column vectors

$$\mathbf{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}, \tag{A.1}$$

whose entries are the components in an n-dimensional Cartesian reference and may depend on position, time, and other parameters. The *scalar product* of the two vectors is indicated with $\mathbf{a} \cdot \mathbf{b}$ and is defined as

$$\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^{n} a_i^* b_i . \tag{A.2}$$

with a_i^* the complex conjugate of a_i. Two non-vanishing vectors $\mathbf{a}$ and $\mathbf{b}$ are *orthogonal* if $\mathbf{a} \cdot \mathbf{b} = 0$. As $\mathbf{b} \cdot \mathbf{a} = (\mathbf{a} \cdot \mathbf{b})^*$, the order of the factors in the scalar product matters; in fact it becomes irrelevant only when the factors are real. The scalar product is distributive and bilinear; if, say, $\mathbf{a} = h_1\,\mathbf{p}_1 + h_2\,\mathbf{p}_2$, then

$$\mathbf{a} \cdot (k_1\,\mathbf{b}_1 + k_2\,\mathbf{b}_2) = h_1^*\,k_1\,\mathbf{p}_1 \cdot \mathbf{b}_1 + h_2^*\,k_1\,\mathbf{p}_2 \cdot \mathbf{b}_1 + h_1^*\,k_2\,\mathbf{p}_1 \cdot \mathbf{b}_2 + h_2^*\,k_2\,\mathbf{p}_2 \cdot \mathbf{b}_2, \tag{A.3}$$

where h_1, h_2, k_1, k_2 are complex constants (in (A.3), the product $k_1\,\mathbf{b}_1$ is the vector of components $k_1\,b_{1i}$, and so on). The *modulus* of $\mathbf{a}$ is defined as

$$a = |\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}} = \left(\sum_{i=1}^{n} |a_i|^2 \right)^{1/2} \geq 0. \tag{A.4}$$

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A.2 Schwarz Inequality and Generalizations

Using (A.2, A.3, A.4) one proves the *Schwarz inequality*

$$|\mathbf{a} \cdot \mathbf{b}| \le a\, b. \tag{A.5}$$

The above is obvious if $\mathbf{a} = 0$ or $\mathbf{b} = 0$; let $\mathbf{b} \neq 0$ and define $\mathbf{c} = \mathbf{a} - (\mathbf{a} \cdot \mathbf{b})\, \mathbf{b}/b^2$, whence $\mathbf{c} \cdot \mathbf{b} = 0$. It follows

$$a^2 = \left(\mathbf{c} + \frac{\mathbf{a} \cdot \mathbf{b}}{b^2}\, \mathbf{b}\right) \cdot \left(\mathbf{c} + \frac{\mathbf{a} \cdot \mathbf{b}}{b^2}\, \mathbf{b}\right) = c^2 + \frac{|\mathbf{a} \cdot \mathbf{b}|^2}{b^2} \ge \frac{|\mathbf{a} \cdot \mathbf{b}|^2}{b^2}, \tag{A.6}$$

which is equivalent to (A.5). The strict equality in (A.5) holds if and only if $\mathbf{b} = k\, \mathbf{a}$, with k any complex constant. Observing that $|\mathbf{a} \cdot \mathbf{b}|^2 = \Re^2(\mathbf{a} \cdot \mathbf{b}) + \Im^2(\mathbf{a} \cdot \mathbf{b})$, from (A.5) one also derives the inequalities $-ab \le \Re(\mathbf{a} \cdot \mathbf{b}) \le +ab$. Thanks to this, one defines the cosine of the angle ϑ between two non-vanishing vectors $\mathbf{a}$ and $\mathbf{b}$ as

$$\cos \vartheta = \frac{\Re(\mathbf{a} \cdot \mathbf{b})}{ab}. \tag{A.7}$$

Other types of products may be defined besides the scalar product, also involving higher-rank factors: for instance, $n \times n$ matrices of the second rank like

$$\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{bmatrix}, \qquad \mathbf{B} = \begin{bmatrix} B_{11} & B_{12} & \dots & B_{1n} \\ B_{21} & B_{22} & \dots & B_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ B_{n1} & B_{n2} & \dots & B_{nn} \end{bmatrix}, \tag{A.8}$$

and so on. Given a second-rank matrix $\mathbf{A}$ of entries A_{ij}, its *transpose* $\mathbf{Q} = \mathbf{A}^T$ is the matrix of entries $Q_{ij} = A_{ji}$. Transposition applies also to vectors: the transpose of the column vector $\mathbf{a}$ defined in (A.1) is the row vector $\mathbf{a}^T = [a_1, \dots, a_n]$. With these premises, given the column vectors $\mathbf{a}$, $\mathbf{b}$ and the matrices $\mathbf{A}$, $\mathbf{B}$, the products $\mathbf{A}\,\mathbf{B}$, $\mathbf{A}\,\mathbf{b}$, and $\mathbf{a}\,\mathbf{b}^T$ yield, respectively, an $n \times n$ matrix, an n-dimensional column vector, and an $n \times n$ matrix whose entries are

$$(\mathbf{A}\,\mathbf{B})_{ij} = \sum_{k=1}^{n} A_{ik}\, B_{kj}, \qquad (\mathbf{A}\,\mathbf{b})_i = \sum_{j=1}^{n} A_{ij}\, b_j, \qquad \left(\mathbf{a}\,\mathbf{b}^T\right)_{ij} = a_i\, b_j. \tag{A.9}$$

Applying definitions (A.9) one finds

$$(\mathbf{A}\,\mathbf{B})^T = \mathbf{B}^T \mathbf{A}^T, \qquad (\mathbf{A}\,\mathbf{b})^T = \mathbf{b}^T \mathbf{A}^T, \qquad \left(\mathbf{a}\,\mathbf{b}^T\right)^T = \mathbf{b}\,\mathbf{a}^T. \tag{A.10}$$

A.3 *Nabla* Operator

A further extension of the concepts introduced in this chapter consists in replacing one or more factors with an operator. An important example is that of the real, vector operator *nabla*,[1]

$$\nabla = \begin{bmatrix} \partial/\partial x_1 \\ \vdots \\ \partial/\partial x_n \end{bmatrix}, \tag{A.11}$$

where $x_1, \dots, x_n$ are the coordinates of an n-dimensional Cartesian reference. The product of ∇ and a complex, scalar function $f(x_1, \dots, x_n)$ is defined in the same manner as the product of a vector and a scalar quantity introduced above: ∇f is a vector of components $(\nabla)_i f$, namely,

$$\nabla f = \begin{bmatrix} \partial f/\partial x_1 \\ \vdots \\ \partial f/\partial x_n \end{bmatrix}. \tag{A.12}$$

In turn, the scalar product of ∇ and a complex vector $\mathbf{a}$ of the same dimension as ∇ yields

$$\nabla \cdot \mathbf{a} = \frac{\partial a_1}{\partial x_1} + \ldots + \frac{\partial a_n}{\partial x_n}. \tag{A.13}$$

The product defined by (A.12) is also called *gradient* of f, whereas the scalar product (A.13) is also called *divergence* of $\mathbf{a}$. The corresponding symbols are $\nabla f = \operatorname{grad} f$ and $\nabla \cdot \mathbf{a} = \operatorname{div} \mathbf{a}$, respectively. The scalar product of ∇ by itself is called *Laplacian operator*

$$\nabla^2 = \nabla \cdot \nabla = \frac{\partial^2}{\partial x_1^2} + \ldots + \frac{\partial^2}{\partial x_n^2}, \tag{A.14}$$

then,

$$\nabla^2 f = \frac{\partial^2 f}{\partial x_1^2} + \ldots + \frac{\partial^2 f}{\partial x_n^2}, \qquad \nabla^2 \mathbf{a} = \begin{bmatrix} \nabla^2 a_1 \\ \vdots \\ \nabla^2 a_n \end{bmatrix}. \tag{A.15}$$

Combining the above definitions yields the identities

$$\nabla^2 f = \nabla \cdot (\nabla f) = \operatorname{div} \operatorname{grad} f, \quad \nabla \cdot (f^* \mathbf{a}) = \operatorname{div} (f^* \mathbf{a}) = f^* \operatorname{div} \mathbf{a} + \operatorname{grad} f \cdot \mathbf{a}. \tag{A.16}$$

[1] Symbol ∇ is *not* a Greek letter. However, the term *nabla* is a Greek word, meaning "harp".

If, in turn, it is $\mathbf{a} = \operatorname{grad} g$, the second relation of (A.16) with the aid of the first one yields the identity

$$\operatorname{div}(f^* \operatorname{grad} g) = f^* \nabla^2 g + \operatorname{grad} f \cdot \operatorname{grad} g. \tag{A.17}$$

A.4 Dyadic Products

Sometimes it is convenient to adopt a notation that uses the basis set of real, mutually-orthogonal unit vectors $\mathbf{i}_1, \ldots, \mathbf{i}_n$ associated with the axes of a Cartesian reference. By construction it is $\mathbf{i}_r \cdot \mathbf{i}_s = \delta_{rs}$, where the *Kronecker symbol* δ_{rs} is the entry of indices rs of a second-rank matrix defined as

$$\delta_{rs} = \begin{cases} 1 & s = r \\ 0 & s \neq r \end{cases} \tag{A.18}$$

The expression of vector $\mathbf{a}$ in terms of the basis vectors is $\mathbf{a} = a_1 \mathbf{i}_1 + \ldots + a_n \mathbf{i}_n$. The notation applies also to the higher-rank objects; for instance, in this notation the matrix $\mathbf{A}$ of (A.8) reads

$$\mathbf{A} = A_{11} \mathbf{i}_1 \mathbf{i}_1^T + A_{12} \mathbf{i}_1 \mathbf{i}_2^T + \ldots + A_{n,n-1} \mathbf{i}_n \mathbf{i}_{n-1}^T + A_{nn} \mathbf{i}_n \mathbf{i}_n^T, \tag{A.19}$$

A group like $\mathbf{i}_r \mathbf{i}_s^T$ is also called *dyadic product*. Observing that $\mathbf{i}_r$ is an n-dimensional column vector whose rth entry is equal to 1 while all the other entries are equal to 0, the application of the third equation in (A.9) shows that $\mathbf{i}_r \mathbf{i}_s^T$ is an $n \times n$ matrix whose entry of indices rs is equal to 1, while all the other entries are equal to zero. As a consequence, the form (A.19) expresses $\mathbf{A}$ as a sum of matrices, each associated to an individual entry. Using this notation, a product like $\mathbf{A}\,\mathbf{b}$ reads $\sum_{rs} A_{rs} \mathbf{i}_r \mathbf{i}_s^T \sum_k b_k \mathbf{i}_k$. On the other hand, due to the second equation in (A.9), the same product is equal to $\sum_{rs} A_{rs} b_s \mathbf{i}_r$. This shows that $\mathbf{i}_r \mathbf{i}_s^T \mathbf{i}_k = \mathbf{i}_r \delta_{sk}$, that is, the juxtaposition of the right unit vector of the dyadic product with the next unit vector must be treated as a scalar product.

The relation defined by the second equation in (A.9) applies also when $\mathbf{b}$ is replaced with a vector operator, with the provision that the operator is meant to act towards the left. For instance, replacing $\mathbf{b}$ with ∇ yields $(\mathbf{A}\,\nabla)_i = \sum_{j=1}^n \partial A_{ij}/\partial x_j$. It follows that the divergence of a second-rank matrix is a column vector of the form

$$\operatorname{div} \mathbf{A} = \sum_{j=1}^{n} \frac{\partial A_{1j}}{\partial x_j} \mathbf{i}_1 + \ldots + \sum_{j=1}^{n} \frac{\partial A_{nj}}{\partial x_j} \mathbf{i}_n. \tag{A.20}$$

In turn, considering the product defined by the third equation in (A.9) and replacing $\mathbf{b}$ with ∇, still with the provision that the operator acts towards the left, yields $(\mathbf{a}\,\nabla^T)_{ij} = \partial a_i/\partial x_j$. It follows that the gradient of a column vector is a second-rank matrix of the form

$$\operatorname{grad} \mathbf{a} = \frac{\partial a_1}{\partial x_1} \mathbf{i}_1 \mathbf{i}_1^T + \frac{\partial a_1}{\partial x_2} \mathbf{i}_1 \mathbf{i}_2^T + \ldots + \frac{\partial a_n}{\partial x_{n-1}} \mathbf{i}_1 \mathbf{i}_{n-1}^T + \frac{\partial a_n}{\partial x_n} \mathbf{i}_n \mathbf{i}_n^T \tag{A.21}$$

whence, from (A.20),

$$\mathrm{div}\,(f\,\mathbf{A}) = f\ \mathrm{div}\,\mathbf{A} + \mathbf{A}\ \mathrm{grad}\, f, \qquad \mathrm{div}\,(\mathbf{a}\,\mathbf{b}^T) = \mathbf{a}\ \mathrm{div}\,\mathbf{b} + (\,\mathrm{grad}\,\mathbf{a})\,\mathbf{b}. \tag{A.22}$$

A.5 Divergence Theorem

The *divergence theorem* (or *Gauss theorem*) states that

$$\int_V \mathrm{div}\,\mathbf{v}\,\mathrm{d}V = \int_S \mathbf{n}\cdot\mathbf{v}\,\mathrm{d}S, \tag{A.23}$$

where V is an n-dimensional volume, $\mathrm{d}V = \mathrm{d}x_1 \ldots \mathrm{d}x_n$, S the $(n-1)$-dimensional surface enclosing V, and $\mathbf{n}$ the unit vector normal to the surface element $\mathrm{d}S$, oriented in the outward direction with respect to S. Letting $\mathbf{v} = f^*\ \mathrm{grad}\, g$ and using (A.17) yields the *first Green theorem*

$$\int_S f^*\,\frac{\partial g}{\partial n}\,\mathrm{d}S = \int_V \left(f^*\,\nabla^2 g + \mathrm{grad}\, f\cdot\mathrm{grad}\, g\right)\,\mathrm{d}V, \tag{A.24}$$

where $\partial g/\partial n = \mathbf{n}\cdot\mathrm{grad}\, g$ is the derivative of g in the direction of $\mathbf{n}$. It is easily found that (A.24) is the generalization to n dimensions of the integration by parts. Rewriting (A.24) after letting $\mathbf{v} = g\ \mathrm{grad}\, f^*$, and subtracting from (A.24), yields the *second Green theorem*

$$\int_S \left(f^*\,\frac{\partial g}{\partial n} - g\,\frac{\partial f^*}{\partial n}\right)\,\mathrm{d}S = \int_V \left(f^*\,\nabla^2 g - g\nabla^2 f^*\right)\,\mathrm{d}V. \tag{A.25}$$

A special case of the first Green theorem occurs when vector $\mathbf{b} = \mathrm{grad}\, g$ is constant; the relation (A.24) then reduces to

$$\int_S f^*\,\mathbf{n}\,\mathrm{d}S\ \cdot\mathbf{b} = \int_V \mathrm{grad}\, f\,\mathrm{d}V\ \cdot\mathbf{b}, \qquad \mathbf{b} = \mathrm{const}. \tag{A.26}$$

As identity (A.26) holds for any choice of $\mathbf{b}$, the two integrals in it are equal to each other.

A.6 Vector Product

Another possible product between two vectors is the *vector product* $\mathbf{a}\wedge\mathbf{b}$, which yields a column vector. In contrast with the other products introduced in this section, the definition of the vector product will be limited to the three-dimensional case; it is given as the expansion of a determinant, namely,

$$\mathbf{a}\wedge\mathbf{b} = \begin{bmatrix} \mathbf{i}_1 & \mathbf{i}_2 & \mathbf{i}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix} \quad\Rightarrow\quad \mathbf{a}\wedge\mathbf{b} = \begin{bmatrix} a_2 b_3 - a_3 b_2 \\ a_3 b_1 - a_1 b_3 \\ a_1 b_2 - a_2 b_1 \end{bmatrix}. \tag{A.27}$$

From (A.27) it follows $\mathbf{b} \wedge \mathbf{a} = -\mathbf{a} \wedge \mathbf{b}$ and $\mathbf{a} \wedge \mathbf{a} = 0$. The latter also shows that, if two non-vanishing vectors are parallel to each other, say, $\mathbf{b} = k\,\mathbf{a} \neq 0$, then $\mathbf{a} \wedge \mathbf{b} = 0$. When the vector product involves the unit vectors associated to the axes of a right-handed Cartesian reference, the following relations are found:

$$\mathbf{i}_1 \wedge \mathbf{i}_2 = \mathbf{i}_3, \qquad \mathbf{i}_2 \wedge \mathbf{i}_3 = \mathbf{i}_1, \qquad \mathbf{i}_3 \wedge \mathbf{i}_1 = \mathbf{i}_2. \tag{A.28}$$

An intrinsic relation that provides the modulus of $\mathbf{a} \wedge \mathbf{b}$ is found by specifying (A.7) for the case of three-dimensional, real vectors, this yielding

$$\cos^2 \vartheta = 1 - \sin^2 \vartheta = \frac{\left(\sum_{i=1}^{3} a_i\, b_i\right)^2}{a^2\, b^2}. \tag{A.29}$$

As $\cos \vartheta = 1$ when the two vectors are parallel, $\mathbf{b} = k\,\mathbf{a}$, $k > 0$, while $\cos \vartheta = -1$ when they are antiparallel, $\mathbf{b} = k\,\mathbf{a}$, $k < 0$, the range of ϑ is $[0, \pi]$. Letting $r_{ij} = a_i\, b_j - a_j\, b_i$ and observing that $(\sum_{i=1}^{3} a_i^2)(\sum_{i=1}^{3} b_i^2) = (\sum_{i=1}^{3} a_i\, b_i)^2 + r_{23}^2 + r_{31}^2 + r_{12}^2$ provides

$$\sin^2 \vartheta = \frac{r_{23}^2 + r_{31}^2 + r_{12}^2}{a^2\, b^2} = \frac{|\mathbf{a} \wedge \mathbf{b}|^2}{a^2\, b^2}, \qquad |\mathbf{a} \wedge \mathbf{b}| = a\, b\, \sin \vartheta, \tag{A.30}$$

where $\sin \vartheta \geq 0$ due to the range of ϑ.

A.7 Mixed Product

The vector product $\mathbf{a} \wedge \mathbf{b}$ can in turn be scalarly multiplied by another vector $\mathbf{c}$, to yield a scalar quantity called *mixed product*. For the sake of simplicity, in the definition of the mixed product the three vectors will be considered real. From (A.2) one finds

$$\mathbf{a} \wedge \mathbf{b} \cdot \mathbf{c} = \sum_{i=1}^{3} (\mathbf{a} \wedge \mathbf{b})_i\; c_i = \begin{vmatrix} c_1 & c_2 & c_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix}. \tag{A.31}$$

The two determinants in (A.31) are equal because they transform into each other by interchanging rows an even number of times. On the other hand, from their equality it follows $\mathbf{a} \wedge \mathbf{b} \cdot \mathbf{c} = \mathbf{a} \cdot \mathbf{b} \wedge \mathbf{c}$, namely, the mixed product is invariant upon interchange of the “wedge” and “dot” symbols.

Considering three non-vanishing vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, where $\mathbf{a}$ and $\mathbf{b}$ are not parallel to each other, and remembering the properties of determinants, one finds that the mixed product vanishes if $\mathbf{c}$ is parallel to $\mathbf{a}$ or parallel to $\mathbf{b}$. In fact,

$$\mathbf{a} \wedge \mathbf{b} \cdot \mathbf{a} = \mathbf{a} \wedge \mathbf{b} \cdot \mathbf{b} = 0. \tag{A.32}$$

It follows that the vector product $\mathbf{a} \wedge \mathbf{b}$ is normal to both $\mathbf{a}$ and $\mathbf{b}$, namely, is normal to the plane defined by the two non-parallel vectors $\mathbf{a}$ and $\mathbf{b}$. If one associates the plane of $\mathbf{a}$ and $\mathbf{b}$ with that of the unit vectors $\mathbf{i}_1$ and $\mathbf{i}_2$ then, using (A.28), the vector product simplifies to $\mathbf{a} \wedge \mathbf{b} = (a_1 b_2 - a_2 a_1) \mathbf{i}_3$, that provides the information about the direction of $\mathbf{a} \wedge \mathbf{b}$. Finally, using (A.27) twice provides the expression for the *double vector product*

$$\mathbf{a} \wedge (\mathbf{b} \wedge \mathbf{c}) = \mathbf{a} \cdot \mathbf{c}\, \mathbf{b} - \mathbf{a} \cdot \mathbf{b}\, \mathbf{c}, \qquad (\mathbf{a} \wedge \mathbf{b}) \wedge \mathbf{c} = \mathbf{a} \cdot \mathbf{c}\, \mathbf{b} - \mathbf{b} \cdot \mathbf{c}\, \mathbf{a}. \tag{A.33}$$

A.8 Rotational of a Vector

The expressions involving the vector product can be extended to the case where one or two vectors are replaced with the nabla operator (A.11). The vector product

$$\nabla \wedge \mathbf{a} = \begin{bmatrix} \mathbf{i}_1 & \mathbf{i}_2 & \mathbf{i}_3 \\ \partial/\partial x_1 & \partial/\partial x_2 & \partial/\partial x_3 \\ a_1 & a_2 & a_3 \end{bmatrix} = \begin{bmatrix} \partial a_3/\partial x_2 - \partial a_2/\partial x_3 \\ \partial a_1/\partial x_3 - \partial a_3/\partial x_1 \\ \partial a_2/\partial x_1 - \partial a_1/\partial x_2 \end{bmatrix} \tag{A.34}$$

is also called *rotational* of $\mathbf{a}$, the corresponding symbol being $\nabla \wedge \mathbf{a} = \mathrm{rot}\, \mathbf{a}$. Combining (A.34) with the three-dimensional case of (A.12) and (A.13) shows that the following identities hold:

$$\mathrm{rot}\,(f\, \mathbf{a}) = f\, \mathrm{rot}\, \mathbf{a} + \mathrm{grad}\, f \wedge \mathbf{a}, \qquad \mathrm{rot}\, \mathrm{grad}\, f = 0, \qquad \mathrm{div}\, \mathrm{rot}\, \mathbf{a} = 0, \tag{A.35}$$

$$\mathrm{rot}\, \mathrm{rot}\, \mathbf{a} = \mathrm{grad}\, \mathrm{div}\, \mathbf{a} - \nabla^2 \mathbf{a}, \qquad \mathrm{div}\,(\mathbf{a} \wedge \mathbf{b}) = \mathbf{b} \cdot \mathrm{rot}\, \mathbf{a} - \mathbf{a} \cdot \mathrm{rot}\, \mathbf{b}. \tag{A.36}$$

Integrating the second equation in (A.36) over a three-dimensional volume V and using (A.23) yields the identity

$$\int_S \mathbf{n} \cdot \mathbf{a} \wedge \mathbf{b}\, \mathrm{d}S = \int_V (\mathbf{b} \cdot \mathrm{rot}\, \mathbf{a} - \mathbf{a} \cdot \mathrm{rot}\, \mathbf{b})\, \mathrm{d}V. \tag{A.37}$$

A special case of (A.37) occurs when vector $\mathbf{a}$ is constant. In fact, noting that $\mathbf{n} \cdot \mathbf{a} \wedge \mathbf{b} = -\mathbf{n} \cdot \mathbf{b} \wedge \mathbf{a} = -\mathbf{n} \wedge \mathbf{b} \cdot \mathbf{a}$, (A.37) reduces to

$$\mathbf{a} \cdot \int_S \mathbf{n} \wedge \mathbf{b}\, \mathrm{d}S = \mathbf{a} \cdot \int_V \mathrm{rot}\, \mathbf{b}\, \mathrm{d}V, \qquad \mathbf{a} = \mathrm{const}. \tag{A.38}$$

As identity (A.38) holds for any choice of $\mathbf{a}$, the two integrals in it are equal to each other.

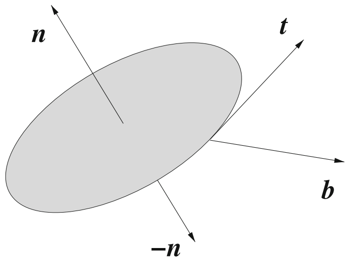

Fig. A.1 Rotational theorem (Sect. A.9): orientation of the unit vectors

A.9 Rotational Theorem

The *rotational theorem* (or *Stokes theorem*) states that

$$\int_S \mathbf{n} \cdot \mathrm{rot}\,\mathbf{v}\,\mathrm{d}S = \int_C \mathbf{t} \cdot \mathbf{v}\,\mathrm{d}C, \tag{A.39}$$

where C is the boundary curve of the open surface S, $\mathbf{t}$ the unit vector tangent to C, and $\mathbf{n}$ the unit vector normal to the surface element $\mathrm{d}S$. The direction of the unit vectors is such that the orientation of $\mathbf{b} = \mathbf{t} \wedge \mathbf{n}$ is external with respect to the curve (Fig. A.1).

A.10 Helmholtz Theorem

A vector $\mathbf{u}$ such that $\mathrm{rot}\,\mathbf{u} = 0$ is called *irrotational*. From the second identity in (A.35) one finds that, if $\mathbf{u} = \mathrm{grad}\, f$, then $\mathbf{u}$ is irrotational. The inverse is not true in general; however, if the domain of $\mathbf{u}$ is simply connected, the condition $\mathrm{rot}\,\mathbf{u} = 0$ implies that $\mathbf{u}$ can be expressed as a gradient: $\mathbf{u} = \mathrm{grad}\, f$.

A vector $\mathbf{v}$ such that $\mathrm{div}\,\mathbf{v} = 0$ is called *solenoidal*. From the third identity in (A.35) one finds that, if $\mathbf{v} = \mathrm{rot}\,\mathbf{a}$, then $\mathbf{v}$ is solenoidal. The inverse is not true in general; however, if the domain of $\mathbf{v}$ is simply connected, the condition $\mathrm{div}\,\mathbf{v} = 0$ implies that $\mathbf{v}$ can be expressed as a rotational: $\mathbf{v} = \mathrm{rot}\,\mathbf{a}$.

The *Helmholtz theorem* states that a vector $\mathbf{w}$ defined in a simply-connected domain can be expressed in a unique manner as the sum of an irrotational and a solenoidal vector:

$$\mathbf{w} = \mathrm{grad}\, f + \mathrm{rot}\,\mathbf{a}. \tag{A.40}$$

Scalar f is found by taking the divergence of both sides of (A.40) and using the identities $\mathrm{div}\,\mathrm{grad}\, f = \nabla^2 f$, $\mathrm{div}\,\mathrm{rot}\,\mathbf{a} = 0$. In turn, vector $\mathbf{a}$ is found by taking the rotational of both sides of (A.40) and using the first identity in (A.36) along with the auxiliary condition $\mathrm{div}\,\mathbf{a} = 0$. By this procedure it is found that f and $\mathbf{a}$ fulfill the relations

$$\nabla^2 f = \mathrm{div}\,\mathbf{w}, \qquad \nabla^2 \mathbf{a} = -\,\mathrm{rot}\,\mathbf{w}. \tag{A.41}$$

The right hand sides of (A.41) are known because $\mathbf{w}$ is prescribed. As a consequence, the problem of finding f and $\mathbf{a}$ is equivalent to solving a set of Poisson equations. The solution of (A.41) is unique provided that $\mathbf{w}$ vanishes at infinity faster than r^{-1} [65, Sect. XI.3]. Unless some additional prescriptions are imposed on f and $\mathbf{a}$, (A.40) still holds if one adds to f an arbitrary constant and, to $\mathbf{a}$, the gradient of an arbitrary scalar function.

A.11 Doubly-Stochastic Matrices

Consider a set of M square matrices of order M, $\mathbf{S}_1, \ldots, \mathbf{S}_M$, and a set of M real, non-negative numbers θ_k such that $\theta_1 + \ldots + \theta_M = 1$. The matrix

$$\mathbf{S} = \sum_{k=1}^{M} \theta_k \mathbf{S}_k \tag{A.42}$$

is called *convex combination* of the $\mathbf{S}_k$ matrices.

The following theorem is easily proved: if the matrices $\mathbf{S}_k$ are doubly stochastic,[2] then $\mathbf{S}$ is doubly stochastic as well. In fact from the definition of $\mathbf{S}$ it is $(\mathbf{S})_{ij} = \sum_{k=1}^{M} \theta_k (\mathbf{S}_k)_{ij}$ whence, adding the terms row-wise,

$$\sum_{j=1}^{M} (\mathbf{S})_{ij} = \sum_{k=1}^{M} \theta_k \sum_{j=1}^{M} (\mathbf{S}_k)_{ij} = \sum_{k=1}^{M} \theta_k = 1. \tag{A.43}$$

The same result is obtained when summing column-wise. As permutation matrices are doubly stochastic, from the above theorem the special case follows: a convex combination of permutation matrices is a doubly-stochastic matrix. The inverse property also holds: a doubly-stochastic matrix is a convex combination of permutation matrices [5].

A.12 Wronskian Determinant

The Wronskian determinant provides the condition of linear independence of functions [51, Sect. 5.2]. Although its properties hold for any number of functions, they will be discussed here for the case of two functions only, say, u and v defined on some interval of the independent variable x. It is convenient to seek for the condition of linear dependence first. If u, v are linearly dependent, then two non-vanishing constants c_1, c_2 exist such that

$$c_1\, u + c_2\, v = 0 \tag{A.44}$$

[2] The definition of doubly-stochastic matrix is given in Sect. 7.6.1.

for all x in the interval. If (A.44) holds, it is easily found that both c_1 and c_2 must differ from zero. Also, as the function at the left hand side of (A.44) vanishes identically, its derivative vanishes as well. Such a derivative exists because u and v are supposed to be solutions of a second-order differential equation. Then,

$$c_1\, u' + c_2\, v' = 0 \tag{A.45}$$

for all x in the interval. As (A.44, A.45) hold together, for all x the two constants c_1, c_2 are the non-trivial solution of a homogeneous algebraic system. Now, if the non-trivial solution of the algebraic system exists for all x, the determinant $W = u\, v' - u'\, v$ must vanish identically. That is, the condition $W = 0$ (identically) is necessary for the linear dependence of u, v. As a consequence, the condition $W \neq 0$ (identically) is sufficient for the linear independence of u, v.

Appendix B
Coordinates

B.1 Spherical Coordinates

When the problem in hand has a spherical symmetry it is convenient to describe the position of a particle by means of the *spherical coordinates*.

With reference to Fig. B.1, the transformation relations between the Cartesian (x, y, z) and spherical (r, ϑ, φ) coordinates are

$$\begin{cases} x = r \sin\vartheta \cos\varphi \\ y = r \sin\vartheta \sin\varphi \\ z = r \cos\vartheta \end{cases} \qquad \begin{cases} r^2 = x^2 + y^2 + z^2 \\ \cos\vartheta = z/r \\ \tan\varphi = y/x \end{cases} \tag{B.1}$$

that are a special case of (1.26). The limits of the spherical coordinates are $0 \le r < \infty$, $0 \le \vartheta \le \pi$, $0 \le \varphi < 2\pi$. The 3×3 matrix of the partial derivatives of the Cartesian coordinates with respect to the spherical ones, expressed in terms of the latter (*Jacobian matrix*), is

$$\frac{\partial(x, y, z)}{\partial(r, \vartheta, \varphi)} = \begin{bmatrix} \sin\vartheta \cos\varphi & r \cos\vartheta \cos\varphi & -r \sin\vartheta \sin\varphi \\ \sin\vartheta \sin\varphi & r \cos\vartheta \sin\varphi & r \sin\vartheta \cos\varphi \\ \cos\vartheta & -r \sin\vartheta & 0 \end{bmatrix}, \tag{B.2}$$

where the left hand side is a short-hand notation for a matrix whose elements are $J_{11} = \partial x/\partial r$, $J_{12} = \partial x/\partial\vartheta$, and so on. The *Jacobian determinant* is

$$J = \det \frac{\partial(x, y, z)}{\partial(r, \vartheta, \varphi)} = r^2 \sin\vartheta. \tag{B.3}$$

The matrix of the partial derivatives of the spherical coordinates with respect to the Cartesian ones, expressed in terms of the former, is

$$\frac{\partial(r, \vartheta, \varphi)}{\partial(x, y, z)} = \begin{bmatrix} \sin\vartheta \cos\varphi & \sin\vartheta \sin\varphi & \cos\vartheta \\ (1/r) \cos\vartheta \cos\varphi & (1/r) \cos\vartheta \sin\varphi & -(1/r) \sin\vartheta \\ -(1/r) \sin\varphi/\sin\vartheta & (1/r) \cos\varphi/\sin\vartheta & 0 \end{bmatrix}, \tag{B.4}$$

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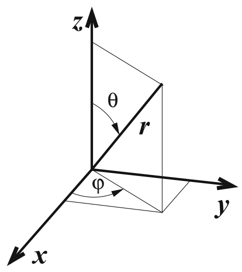

Fig. B.1 Cartesian (x, y, z) and spherical (r, ϑ, φ) coordinates

whence

$$\det \frac{\partial(r, \vartheta, \varphi)}{\partial(x, y, z)} = \frac{1}{r^2 \sin\vartheta} = \frac{1}{J}. \tag{B.5}$$

To calculate (B.4) consider, e.g., the last term of the second row, $(\partial\vartheta/\partial z)_{xy} = -(1/r)\sin\vartheta$. The second line of the second group of (B.1) yields $(\partial \cos\vartheta/\partial z)_{xy} = 1/r - z^2/r^3$, where $(\partial r/\partial z)_{xy} = z/r$ has been used, that in turn derives from the first line of the second group of (B.1). The relation $z = r\cos\vartheta$ then yields $(\partial\cos\vartheta/\partial z)_{xy} = (1/r)\sin^2\vartheta$. On the other hand the same quantity can also be written as $(\partial\cos\vartheta/\partial z)_{xy} = -\sin\vartheta\,(\partial\vartheta/\partial z)_{xy}$. Comparing the two expressions above yields the result sought.

Differentiating with respect to time the first of (B.1) yields the relations

$$\begin{cases} \dot{x} = \dot{r}\sin\vartheta\cos\varphi + r\,\dot{\vartheta}\cos\vartheta\cos\varphi - r\,\dot{\varphi}\sin\vartheta\sin\varphi \\ \dot{y} = \dot{r}\sin\vartheta\sin\varphi + r\,\dot{\vartheta}\cos\vartheta\sin\varphi + r\,\dot{\varphi}\sin\vartheta\cos\varphi \\ \dot{z} = \dot{r}\cos\vartheta - r\,\dot{\vartheta}\sin\vartheta \end{cases} \tag{B.6}$$

that express the components of the velocity in the Cartesian reference as functions of the generalized coordinates r, ϑ, φ and generalized velocities $\dot{r}, \dot{\vartheta}, \dot{\varphi}$ of the spherical reference. From (B.6) the expression of the kinetic energy in spherical coordinates follows:

$$T = \frac{1}{2} m\,(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) = \frac{1}{2} m\,\left(\dot{r}^2 + r^2\dot{\vartheta}^2 + r^2\dot{\varphi}^2\sin^2\vartheta\right). \tag{B.7}$$

B.2 Polar Coordinates

To describe the motion of particles confined over a plane one may adopt, instead of the Cartesian coordinates x, y, the *polar coordinates* r, φ. The relations between the two groups of coordinates are

$$\begin{cases} x &= r\cos\varphi \\ y &= r\sin\varphi \end{cases} \qquad \begin{cases} r^2 &= x^2+y^2 \\ \tan\varphi &= y/x \end{cases} \tag{B.8}$$

The limits of the polar coordinates are $0 \le r < \infty$, $0 \le \varphi < 2\pi$. The Jacobian matrix and the Jacobian determinant are, respectively,

$$\frac{\partial(x,y)}{\partial(r,\varphi)} = \begin{bmatrix} \cos\varphi & -r\sin\varphi \\ \sin\varphi & r\cos\varphi \end{bmatrix}, \qquad J = \det\frac{\partial(x,y)}{\partial(r,\varphi)} = r. \tag{B.9}$$

Differentiating with respect to time the first of (B.8) yields the relations

$$\begin{cases} \dot{x} &= \dot{r}\cos\varphi - r\,\dot{\varphi}\sin\varphi \\ \dot{y} &= \dot{r}\sin\varphi + r\,\dot{\varphi}\cos\varphi \end{cases} \tag{B.10}$$

that express the components of the velocity in the Cartesian reference as functions of the generalized coordinates r, φ and generalized velocities $\dot{r}, \dot{\varphi}$ of the polar reference. From (B.10) the expression of the kinetic energy in polar coordinates follows:

$$T = \frac{1}{2}m\,(\dot{x}^2+\dot{y}^2) = \frac{1}{2}m\,\left(\dot{r}^2 + r^2\dot{\varphi}^2\right). \tag{B.11}$$

B.3 Coordinate Rotation

Consider a coordinate transformation that consists in a rotation around the origin, bringing a right-handed system of coordinates $\mathbf{x} = (x_1, x_2, x_3)$ into another right-handed system $\mathbf{s} = (s_1, s_2, s_3)$. The transformation is described by the linear relations

$$\begin{cases} s_1 &= a_{11}x_1 + a_{12}x_2 + a_{13}x_3 \\ s_2 &= a_{21}x_1 + a_{22}x_2 + a_{23}x_3 \\ s_3 &= a_{31}x_1 + a_{32}x_2 + a_{33}x_3 \end{cases} \tag{B.12}$$

which can be recast in the matrix form $\mathbf{s} = \mathbf{A}\mathbf{x}$. It is known that a matrix describing this type of transformation is *orthogonal* [42, Sect. 4.2], namely,

$$\sum_{i=1}^{3} a_{ij}\,a_{ik} = \delta_{jk}, \qquad \det\mathbf{A} = 1, \qquad \mathbf{A}^{-1} = \mathbf{A}^T, \qquad j,k = 1,2,3, \tag{B.13}$$

where apex T indicates the transpose. From (B.13) it follows $\left(\mathbf{A}^{-1}\right)^T = \mathbf{A}$. As a consequence, the effect of the rotation onto the modulus of a particle's velocity is found from

$$\left(\dot{\mathbf{x}}^T, \dot{\mathbf{x}}\right) = \left[\left(\mathbf{A}^{-1}\dot{\mathbf{s}}\right)^T, \mathbf{A}^{-1}\dot{\mathbf{s}}\right] = \left(\dot{\mathbf{s}}^T\mathbf{A}, \mathbf{A}^{-1}\dot{\mathbf{s}}\right) = \left(\dot{\mathbf{s}}^T, \mathbf{A}\,\mathbf{A}^{-1}\dot{\mathbf{s}}\right) = \left(\dot{\mathbf{s}}^T, \dot{\mathbf{s}}\right). \tag{B.14}$$

In (B.14) the symbol $(\mathbf{a}^T, \mathbf{b})$ denotes the scalar product between the vectors $\mathbf{a}$ and $\mathbf{b}$, namely, it is equivalent to $\mathbf{a} \cdot \mathbf{b}$. The above calculation shows that $u^2 = (\dot{\mathbf{x}}^T, \dot{\mathbf{x}})$ is invariant under rotation of the coordinate system. The same reasoning applies to the modulus of position $r^2 = (\mathbf{x}^T, \mathbf{x}) = (\mathbf{s}^T, \mathbf{s})$.

B.4 Differential Operators Under Coordinate Transformations

Consider the coordinate transformation between the two sets $x_i, \xi_i, i = 1, 2, \ldots, n$:

$$\xi_i = \xi_i(x_1, \ldots, x_n), \qquad x_i = x_i(\xi_1, \ldots, \xi_n). \tag{B.15}$$

If a function f is transformed using the above, the following hold:

$$\frac{\partial f}{\partial x_i} = \sum_{j=1}^{n} \frac{\partial f}{\partial \xi_j} \frac{\partial \xi_j}{\partial x_i}, \qquad \frac{\partial^2 f}{\partial x_i^2} = \sum_{j=1}^{n} \left(\frac{\partial f}{\partial \xi_j} \frac{\partial^2 \xi_j}{\partial x_i^2} + \sum_{k=1}^{n} \frac{\partial^2 f}{\partial \xi_j \partial \xi_k} \frac{\partial \xi_j}{\partial x_i} \frac{\partial \xi_k}{\partial x_i} \right). \tag{B.16}$$

Adding up over i in the second of (B.16) yields

$$\nabla^2 f = \sum_{j=1}^{n} \left(\frac{\partial f}{\partial \xi_j} \nabla^2 \xi_j + \sum_{k=1}^{n} \frac{\partial^2 f}{\partial \xi_j \partial \xi_k} \nabla \xi_j \cdot \nabla \xi_k \right), \tag{B.17}$$

where symbols ∇ and ∇^2 indicate, respectively, the gradient and the Laplacian operator with respect to the coordinates x_i. By way of example consider the transformation (B.1) from Cartesian to spherical coordinates. Remembering (B.4) one finds

$$\nabla r \cdot \nabla r = 1, \qquad \nabla \vartheta \cdot \nabla \vartheta = \frac{1}{r^2}, \qquad \nabla \varphi \cdot \nabla \varphi = \frac{1}{r^2 \sin^2 \vartheta}, \tag{B.18}$$

$$\nabla r \cdot \nabla \vartheta = 0, \qquad \nabla \vartheta \cdot \nabla \varphi = 0, \qquad \nabla \varphi \cdot \nabla r = 0, \tag{B.19}$$

whence

$$\nabla^2 f = \frac{\partial f}{\partial r} \nabla^2 r + \frac{\partial^2 f}{\partial r^2} + \frac{\partial f}{\partial \vartheta} \nabla^2 \vartheta + \frac{\partial^2 f}{\partial \vartheta^2} \frac{1}{r^2} + \frac{\partial f}{\partial \varphi} \nabla^2 \varphi + \frac{\partial^2 f}{\partial \varphi^2} \frac{1}{r^2 \sin^2 \vartheta}. \tag{B.20}$$

In turn, letting $\gamma \doteq \sin \vartheta \cos \vartheta / r$, $\zeta \doteq \sin \varphi \cos \varphi / r$, $\sigma \doteq \sin^2 \vartheta$, the terms $\nabla^2 r$, $\nabla^2 \vartheta$, $\nabla^2 \varphi$ are found from

$$\begin{bmatrix} \partial^2 r / \partial x^2 & \partial^2 r / \partial y^2 & \partial^2 r / \partial z^2 \\ \partial^2 \vartheta / \partial x^2 & \partial^2 \vartheta / \partial y^2 & \partial^2 \vartheta / \partial z^2 \\ \partial^2 \varphi / \partial x^2 & \partial^2 \varphi / \partial y^2 & \partial^2 \varphi / \partial z^2 \end{bmatrix} = \frac{1}{r} \times \tag{B.21}$$

$$\times \begin{bmatrix} 1-\sigma\cos^2\varphi & 1-\sigma\sin^2\varphi & \sigma \\ \gamma\,(\sin^2\varphi/\sigma-2\cos^2\varphi) & \gamma\,(\cos^2\varphi/\sigma-2\sin^2\varphi) & 2\gamma \\ 2\zeta/\sigma & -2\zeta/\sigma & 0 \end{bmatrix}, \tag{B.22}$$

whence

$$\nabla^2 r = \frac{2}{r}, \qquad \nabla^2\vartheta = \frac{1}{r^2}\frac{\cos\theta}{\sin\theta}, \qquad \nabla^2\varphi = 0, \tag{B.23}$$

$$\nabla^2 f = \frac{\partial f}{\partial r}\frac{2}{r} + \frac{\partial^2 f}{\partial r^2} + \frac{\partial f}{\partial\vartheta}\frac{1}{r^2}\frac{\cos\theta}{\sin\theta} + \frac{\partial^2 f}{\partial\vartheta^2}\frac{1}{r^2} + \frac{\partial^2 f}{\partial\varphi^2}\frac{1}{r^2\sin^2\vartheta} = \tag{B.24}$$

$$= \frac{1}{r}\frac{\partial^2}{\partial r^2}(rf) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\,\frac{\partial f}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2 f}{\partial\varphi^2}. \tag{B.25}$$

B.5 Density of States

Consider a function s that depends on the coordinates u, v, w, and on one or more additional parameters that will collectively be indicated with σ. Let

$$S(\sigma) = \iiint s(u,v,w,\sigma)\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w, \tag{B.26}$$

where the integration is carried out over the whole domain of u, v, w. Next, consider the transformation from the original variables to the new variables α, β, η,

$$\alpha = \alpha(u,v,w), \quad \beta = \beta(u,v,w), \quad \eta = \eta(u,v,w), \quad J = \frac{\partial(u,v,w)}{\partial(\alpha,\beta,\eta)}, \tag{B.27}$$

which is assumed to be invertible, so that the Jacobian determinant J does not vanish. After the transformation is carried out, (B.26) takes the form

$$S(\sigma) = \iiint s(\alpha,\beta,\eta,\sigma)\,|J|\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}\eta. \tag{B.28}$$

It may happen that one is interested in the dependence of s on one of the new variables, say, η, rather than in the details about its dependence on the whole set of new variables. In this case one first carries out the integrals with respect to α and β in (B.28), to find

$$h(\eta,\sigma) = \iint s(\alpha,\beta,\eta,\sigma)\,|J|\,\mathrm{d}\alpha\,\mathrm{d}\beta. \tag{B.29}$$

Then one defines

$$b(\eta) = \iint |J|\,\mathrm{d}\alpha\,\mathrm{d}\beta. \tag{B.30}$$

A function like $b(\eta)$ plays an important role in many physical problems (e.g., Sects. 14.6, 15.8.1, 15.8.2). For this reason, although its derivation in this section is of a purely formal nature, $b(\eta)$ will be called *density of states in* η. Note that the density of states depends only on the structure of the variable transformation (B.27) and (at most) on η. The form of (B.29) and (B.30) shows that the ratio $\bar{s} = h/b$ is a weighed average of $s(\alpha, \beta, \eta, \sigma)$ over the two variables α and β, that uses $|J|$ as weight. Introducing the definition of $\bar{s}$ into (B.28) gives the latter the form

$$S(\sigma) = \int b(\eta)\, \bar{s}(\eta, \sigma)\, \mathrm{d}\eta. \tag{B.31}$$

If s happens to be independent of α and β, definition (B.29) yields $h = s\, b$, whence $\bar{s}(\eta, \sigma) = s(\eta, \sigma)$. The derivation of b is not limited to a three-dimensional case; in fact it applies to any number of dimensions. In the following, a few examples in one, two, and three dimensions are given, in which one of the transformation relations (B.27), namely, $\eta = \eta(u, v, w)$, has a quadratic form; these examples are in fact particularly significant for the physical applications, where η stands for the energy and u, v, w stand for the generalized coordinates.

Considering a one-dimensional case with $\eta = u^2$, one finds[3]

$$u = \pm\eta^{1/2}, \qquad |J| = \left|\frac{\partial u}{\partial \eta}\right| = \frac{1}{2}\, \eta^{-1/2}, \qquad b(\eta) = 2\, \frac{1}{2}\, \eta^{-1/2} = \eta^{-1/2}. \tag{B.32}$$

This case is straightforward because there are no other variables involved in the transformation. Instead, in the two-dimensional case with $\eta = u^2 + v^2$, a convenient transformation involving the second variable is of the polar type (B.8), specifically, $u = \eta^{1/2} \cos\varphi$, $v = \eta^{1/2} \sin\varphi$. One finds

$$|J| = \frac{1}{2}, \qquad b(\eta) = \int_0^{2\pi} \frac{1}{2}\, \mathrm{d}\varphi = \pi. \tag{B.33}$$

In the three-dimensional case with $\eta = u^2 + v^2 + w^2$, a convenient transformation involving the other two variables is of the spherical type (B.1), specifically, $u = \eta^{1/2} \sin\vartheta \cos\varphi$, $v = \eta^{1/2} \sin\vartheta \sin\varphi$, $w = \eta^{1/2} \cos\vartheta$. One finds

$$|J| = \frac{1}{2}\, \eta^{1/2} \sin\vartheta, \qquad b(\eta) = \int_0^{2\pi} \int_0^{\pi} \frac{1}{2}\, \eta^{1/2} \sin\vartheta\, \mathrm{d}\vartheta\, \mathrm{d}\varphi = 2\pi\, \eta^{1/2}. \tag{B.34}$$

The above examples show that, despite the fact that the $\eta = \eta(u, v, w)$ relation is quadratic in all cases, the form of $b(\eta)$ changes depending on the number of spatial dimensions.

Still considering the case where one of the transformation relations (B.27) has a quadratic form, the analysis can be extended to arbitrary values of the number

[3] Factor 2 in the last expression of (B.32) accounts for the fact that both positive and negative parts of the segment $[-\,\eta^{1/2}, +\eta^{1/2}]$ must be considered.

of spatial dimensions. As a starting point, and considering provisionally the three-dimensional case, one notes from (B.30) that the following equality holds:[4]

$$B = \int b(\eta)\,\mathrm{d}\eta = \iiint |J|\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}\eta = \iiint \mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w. \qquad \text{(B.35)}$$

Remembering the definition of b, it follows that B is the number of states in the domain of u, v, w. Due to the last integral in (B.34), B is also equal to the volume of such a domain; in turn, due to the first integral, B can be thought of as the sum of the volumes of elementary shells of thickness $\mathrm{d}\eta$, with $b(\eta)$ the area of each shell (that is, the area of the two-dimensional surface $\eta = \text{const}$). These observations provide the key to extending the analysis to the case where η is a quadratic form in an arbitrary number of dimensions,

$$u_1^2 + u_2^2 + \ldots + u_n^2 = \eta, \qquad \eta = g^2. \qquad \text{(B.36)}$$

Letting $\eta = \text{const}$, (B.36) is the equation of an $(n-1)$-dimensional sphere of radius $g \geq 0$ immersed into the n-dimensional space. The problem is thus reduced to expressing the area of the sphere in terms of η; although it can be solved by using a generalization of the spherical coordinates to n dimensions, a more elegant approach consists in finding a recursive expression involving also the sphere's volume.

To this purpose, let V_n indicate the volume of a sphere of an n-dimensional space, and let S_{n-1} indicate the surface area of the same sphere. When $n = 1$, the sphere is a segment whose volume is the length $V_1 = 2g$; for $n = 2$, the sphere is a circle whose volume is the area $V_2 = \pi\,g^2$; for $n = 3$ it is $V_3 = (4/3)\,\pi\,g^3$; for $n = 4$ it is $V_4 = \pi^2\,g^4/2$, and so on; in turn, for $n = 2$ the surface is a circumference whose area is the length $S_1 = 2\,\pi\,g$; for $n = 3$ it is $S_2 = 4\,\pi\,g^2$; for $n = 4$ it is $S_3 = 2\,\pi^2\,g^3$, and so on. Consistently with the expression of B as the integral of b given by (B.35), one finds from the above values the general relation

$$V_n = \frac{g}{n}\,S_{n-1}. \qquad \text{(B.37)}$$

Combining (B.37) with $V_1 = 2g$ also yields $S_0 = 2$, that is, the "surface" of the segment considered above; such a surface is made of the segment's endpoints $\{-1, +1\}$. From (B.37) it also follows that $V_n \propto g^n$ and $S_{n-1} \propto g^{n-1}$, whence $S_n \propto g\,V_{n-1}$ and $V_0 = \text{const}$. From the values found above one finds $S_2/(g\,V_1) = S_3/(g\,V_2) = 2\,\pi$; it follows that $S_n = 2\,\pi\,g\,V_{n-1}$ and $V_0 = 1$. The latter is the "volume" of a sphere in a zero-dimensional space. The recursive relation involving the volumes then reads

$$V_n = \frac{g}{n}\,S_{n-1} = \frac{g}{n}\,2\,\pi\,g\,V_{n-2} = \frac{2\,\pi\,g^2}{n}\,V_{n-2}, \qquad V_0 = 1, \qquad V_1 = 2g. \quad \text{(B.38)}$$

[4] In the practical applications of the concepts illustrated here, the integrands in (B.35) embed a constant factor Q_0, called *density of states in the u, v, w space* which, besides describing some properties of the physical problem under investigation, makes B dimensionless. Here, all variables involved are dimensionless, and Q_0 is set equal to unity.

The above can further by improved by observing that the sequence $V_0, V_1, \ldots$ embeds Euler's Gamma function of half-integer order; in fact, combining (B.37) and (B.38) with the definitions of Sect. C.10, yields

$$V_n = \frac{\pi^{n/2}}{\Gamma(n/2+1)}\, g^n, \qquad S_{n-1} = \frac{n\,\pi^{n/2}}{\Gamma(n/2+1)}\, g^{n-1}. \tag{B.39}$$

The last step consists in expressing the result in terms of η. This is accomplished by noting that $b(\eta)\,\mathrm{d}\eta = S_{n-1}(g)\,\mathrm{d}g$, where $g = \sqrt{\eta}$ and $\mathrm{d}g = \mathrm{d}\sqrt{\eta} = \mathrm{d}\eta/(2\sqrt{\eta})$; then, one finds

$$b(\eta)\,\mathrm{d}\eta = \frac{n\,\pi^{n/2}\eta^{(n-1)/2}}{\Gamma(n/2+1)}\,\frac{\mathrm{d}\eta}{2\eta^{1/2}}, \qquad b(\eta) = \frac{n\,\pi^{n/2}}{2\Gamma(n/2+1)}\,\eta^{n/2-1}. \tag{B.40}$$

Letting $n = 1, 2, 3$ in the second expression of (B.40) renders (B.32), (B.33), (B.34), respectively.

Appendix C
Special Integrals

C.1 Sine Integral

Define the two functions

$$\mathrm{si}(t) = -\frac{\pi}{2} + \int_0^t \frac{\sin x}{x}\,\mathrm{d}x, \qquad N(a) = \int_0^\infty \frac{\sin(ax)}{x}\,\mathrm{d}x. \tag{C.1}$$

The first of them is called *sine integral* and fulfills the limit $\lim_{t\to\infty} \mathrm{si} = 0$, whence $N(1) = \pi/2$. To demonstrate the above one starts from the functions

$$F(y) = \int_0^\infty \exp(-x)\,\frac{\sin(xy)}{x}\,\mathrm{d}x, \quad G(y) = \int_0^\infty \exp(-xy)\,\frac{\sin x}{x}\,\mathrm{d}x, \quad y \ge 0. \tag{C.2}$$

The following hold true: $F(0) = 0$, $G(0) = N(1)$, $F(1) = G(1)$, and

$$\frac{\mathrm{d}F}{\mathrm{d}y} = \int_0^\infty \exp(-x)\,\cos(xy)\,\mathrm{d}x, \qquad \frac{\mathrm{d}G}{\mathrm{d}y} = \int_0^\infty \exp(-xy)\,\sin x\,\mathrm{d}x. \tag{C.3}$$

Integrating (C.3) by parts twice yields $\mathrm{d}F/\mathrm{d}y = 1/(1+y^2)$, $\mathrm{d}G/\mathrm{d}y = -1/(1+y^2)$ whence

$$F(y) = \arctan y + F(0), \quad G(y) = -\arctan y + G(0), \quad 0 \le y < \frac{\pi}{2}. \tag{C.4}$$

It follows $F(1) = F(0) + \pi/4 = \pi/4$ and $F(1) = G(1) = G(0) - \pi/4 = N(1) - \pi/4$. Combining the above yields the result sought. This implicitly proves the convergence of the integrals in (C.1). The calculation of the second of (C.1) is now straightforward and yields

$$N(a) = \begin{cases} -\pi/2, & a < 0, \\ 0, & a = 0, \\ +\pi/2, & a > 0. \end{cases} \tag{C.5}$$

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The integrand in the second of (C.1) is even with respect to x. It follows that an integration carried out from $-\infty$ to $+\infty$ yields $2\,N(a)$. Basing on this one also finds

$$\int_{-\infty}^{+\infty} \frac{\exp(\mathrm{i}\,ax)}{\mathrm{i}\,x}\,\mathrm{d}x = 2\,N(a) + \int_{-\infty}^{+\infty} \frac{\cos(ax)}{\mathrm{i}\,x}\,\mathrm{d}x = 2\,N(a). \tag{C.6}$$

When calculating the second integral in (C.6) one must let $z = \pm ax$, $\epsilon, Z > 0$ and use the principal part. In fact, observing that the integrand is odd one obtains

$$\int_{-\infty}^{+\infty} \frac{\cos(ax)}{\mathrm{i}\,x}\,\mathrm{d}x = \pm\mathrm{i}\lim_{\substack{\epsilon\to 0\\ Z\to\infty}} \left(\int_{-Z}^{-\epsilon} \frac{\cos z}{z}\,\mathrm{d}z + \int_{+\epsilon}^{+Z} \frac{\cos z}{z}\,\mathrm{d}z \right) = 0. \tag{C.7}$$

Combining (C.7) with (C.6) provides an integral representation of the Fourier type for the *step function*

$$H(a) = \left\{ \begin{array}{ll} 0 & a < 0 \\ 1/2 & a = 0 \\ 1 & a > 0 \end{array} \right\} = \frac{1}{2} + \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{\exp(\mathrm{i}ax)}{\mathrm{i}x}\,\mathrm{d}x. \tag{C.8}$$

Still from (C.6), using the identity $2\,\mathrm{i}\,\sin x = \exp(\mathrm{i}\,x) - \exp(-\mathrm{i}\,x)$, one finds

$$\int_{-\infty}^{+\infty} \frac{\sin x}{x} \exp(-\mathrm{i}\,a\,x)\,\mathrm{d}x = N(-a+1) - N(-a-1) = \begin{cases} 0 & |a| > 1 \\ \pi/2 & a = \pm 1 \\ \pi & |a| < 1 \end{cases} \tag{C.9}$$

From (C.9) one derives integrals of a similar form, where $\sin x/x$ is replaced with $\sin^n x/x^n$, $n = 2, 3, \ldots$. The example with $n = 2$ is given below: one starts from

$$\frac{\mathrm{d}}{\mathrm{d}a} \int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} \exp(-\mathrm{i}\,a\,x)\,\mathrm{d}x = \int_{-\infty}^{+\infty} \frac{\sin^2 x}{\mathrm{i}\,x} \exp(-\mathrm{i}\,a\,x)\,\mathrm{d}x, \tag{C.10}$$

and uses the identity $2\,\sin^2 x = 1 - \cos(2\,x)$ to find

$$\int_{-\infty}^{+\infty} \frac{1-\cos(2\,x)}{2\,\mathrm{i}\,x} \exp(-\mathrm{i}\,a\,x)\,\mathrm{d}x = N(-a) + \int_{-\infty}^{+\infty} \frac{\cos(2\,x)}{2\,x} \sin(a\,x)\,\mathrm{d}x, \tag{C.11}$$

where $N(-a)$ derives from (C.6) and the integral on the right hand side is obtained by eliminating the odd part of the integrand. From the identity $\sin[(a+2)\,x] + \sin[(a-2)\,x] = 2\,\sin(a\,x)\,\cos(2\,x)$ such an integral transforms into

$$\int_{-\infty}^{+\infty} \frac{\sin[(a+2)\,x] + \sin[(a-2)\,x]}{4\,x}\,\mathrm{d}x = \frac{1}{2}\,N(a+2) + \frac{1}{2}\,N(a-2), \tag{C.12}$$

where the second definition in (C.1) has been used. Combining (C.10), (C.11), and (C.12) yields

$$\frac{\mathrm{d}}{\mathrm{d}a}\int_{-\infty}^{+\infty}\frac{\sin^2 x}{x^2}\,\exp(-\mathrm{i}\,a\,x)\,\mathrm{d}x=\begin{cases}\pi/2 & -2<a<0\\ -\pi/2 & 0<a<2\\ 0 & |a|>2\end{cases} \tag{C.13}$$

This result shows that the derivative with respect to a of the integral sought is piecewise constant in the interval $-2 < a < +2$, and vanishes elsewhere. The integral is also continuous with respect to a and does not diverge, because $|\sin^2 x/x^2| \le |\sin x/x|$ and (C.9) converges. This reasoning allows one to fix the integration constants, to finally obtain

$$\int_{-\infty}^{+\infty}\frac{\sin^2 x}{x^2}\,\exp(-\mathrm{i}\,a\,x)\,\mathrm{d}x=\begin{cases}(\pi/2)\,(a+2) & -2<a<0\\ -(\pi/2)\,(a-2) & 0<a<2\\ 0 & |a|>2\end{cases} \tag{C.14}$$

By a procedure similar to that used to prove (C.14) one finds

$$\frac{\mathrm{d}}{\mathrm{d}a}\int_{-\infty}^{+\infty}\frac{\sin^2(ax)}{x^2}\,\mathrm{d}x=2\,N(a),\qquad \int_{-\infty}^{+\infty}\frac{\sin^2(ax)}{x^2}\,\mathrm{d}x=\begin{cases}\pi\,a, & a>0\\ -\pi\,a, & a<0\end{cases} \tag{C.15}$$

C.2 Fourier Transform

Let $f(x)$ be a function defined over the entire x axis. Its Fourier transform is defined as the integral

$$G(k)=\mathcal{F}_x f=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}f(x)\,\exp(-\mathrm{i}\,k\,x)\,\mathrm{d}x. \tag{C.16}$$

In turn, the Fourier antitransform is defined as

$$f(x)=\mathcal{F}_x^{-1}G=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}G(k)\,\exp(\mathrm{i}\,k\,x)\,\mathrm{d}k. \tag{C.17}$$

Combining (C.16) and (C.17) provides a representation of f in the form

$$f(x)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp(\mathrm{i}\,k\,x)\left[\int_{-\infty}^{+\infty}f(\xi)\,\exp(-\mathrm{i}\,k\,\xi)\,\mathrm{d}\xi\right]\mathrm{d}k. \tag{C.18}$$

A sufficient condition for the representation (C.18) is

$$\int_{-\infty}^{+\infty}|f(x)|\,\mathrm{d}x<\infty. \tag{C.19}$$

If f is discontinuous of the first kind at some point x_0, the left hand side of (C.18) must be replaced with $[f(x_0^+) + f(x_0^-)]/2$. As the condition (C.19) is sufficient, but not necessary, there are functions that admit an integral representation like (C.18) without fulfilling (C.19). An important example is the unit step function shown in Sect. C.1.

If f depends also on one or more parameters, $f = f(x, u, v, \dots)$, then it is $G = G(k, u, v, \dots)$. In an n-dimensional space, defining the vectors $\mathbf{x} = (x_1, \dots, x_n)$ and $\mathbf{k} = (k_1, \dots, k_n)$, the Fourier transform reads

$$G(\mathbf{k}) = \mathcal{F}_\mathbf{x} f = \frac{1}{(2\,\pi)^{n/2}} \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} f(\mathbf{x}) \exp(-\mathrm{i}\,\mathbf{k}\cdot\mathbf{x})\,\mathrm{d}x_1 \dots \mathrm{d}x_n. \quad \text{(C.20)}$$

A useful relation is found by differentiating both sides of (C.17). To this purpose, one must assume that the conditions for exchanging the derivative with the integral are fulfilled. It is found

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{+\infty} \mathrm{i}\,k\,G(k) \exp(\mathrm{i}kx)\,\mathrm{d}k. \quad \text{(C.21)}$$

Iterating the procedure yields

$$\frac{\mathrm{d}^n f}{\mathrm{d}x^n} = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{+\infty} (\mathrm{i}\,k)^n \; G(k) \exp(\mathrm{i}kx)\,\mathrm{d}k, \quad \text{(C.22)}$$

showing that, if $G(k)$ is the Fourier transform of $f(x)$, then the Fourier transform of $\mathrm{d}^n f/\mathrm{d}x^x$ is $(\mathrm{i}\,k)^n \; G(k)$. Relations like (C.21) and (C.22) are useful, for instance, in the solution of linear differential equations with constant coefficients, because they turn differential relations into polynomial relations (compare with the solution of the diffusion equation carried out in Sect. 23.4).

C.3 Gauss Integral

The relation

$$I_G = \int_0^{+\infty} \exp(-x^2)\,\mathrm{d}x = \int_{-\infty}^{0} \exp(-x^2)\,\mathrm{d}x. \quad \text{(C.23)}$$

is called *Gauss integral* or *Poisson integral*. To calculate its value one may start from the double integral

$$F(R) = \iint_{\Sigma(R)} \exp[-(x^2 + y^2)]\,\mathrm{d}x\mathrm{d}y, \quad \text{(C.24)}$$

where $\Sigma(R)$ is a circle of radius R centered on the origin. Using the polar coordinates (B.8) yields

$$F(R) = \int_0^{2\pi} \mathrm{d}\vartheta \int_0^R \exp(-\rho^2)\,\rho\,\mathrm{d}\rho = \pi\,[1 - \exp(-R^2)], \quad \text{(C.25)}$$

whence $\lim_{R\to\infty} F(R) = \pi$. On the other hand, due to (C.24) it is also

$$\lim_{R\to\infty} F(R) = \iint_{-\infty}^{+\infty} \exp\left[-(x^2+y^2)\right] \mathrm{d}x\,\mathrm{d}y = \lim_{a\to\infty}\left(\int_{-a}^{+a} \exp(-x^2)\,\mathrm{d}x\right)^2. \tag{C.26}$$

Combining (C.25, C.26) with (C.23) provides

$$\int_{-\infty}^{+\infty} \exp(-x^2)\,\mathrm{d}x = \sqrt{\pi}, \qquad I_G = \frac{\sqrt{\pi}}{2}. \tag{C.27}$$

From (C.27) it follows that for any $\lambda > 0$ it is

$$I_0(\lambda) = \int_0^{\infty} \exp(-\lambda x^2)\,\mathrm{d}x = \frac{1}{2}\sqrt{\frac{\pi}{\lambda}}. \tag{C.28}$$

Another integral generated by $\exp(-\lambda x^2)$ is

$$I_1(\lambda) = \int_0^{\infty} x\,\exp(-\lambda x^2)\,\mathrm{d}x = \frac{1}{2\lambda}. \tag{C.29}$$

Thanks to (C.28) and (C.29) it is possible to calculate all integrals of the form

$$I_n(\lambda) = \int_0^{\infty} x^n\,\exp(-\lambda x^2)\,\mathrm{d}x, \qquad n \ge 0. \tag{C.30}$$

In fact, using the recursive relation

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} I_n = \int_0^{\infty} \frac{\partial}{\partial\lambda} x^n\,\exp(-\lambda x^2)\,\mathrm{d}x = -\int_0^{\infty} x^{n+2}\,\exp(-\lambda x^2)\,\mathrm{d}x = -I_{n+2}, \tag{C.31}$$

in combination with (C.29) yields all the integrals whose index is odd,

$$I_{2m+1} = \frac{m!}{2}\,\lambda^{-(m+1)}, \qquad m = 0, 1, 2, \dots . \tag{C.32}$$

Similarly, combining (C.31) with (C.28) yields all the integrals whose index is even,

$$I_{2m}(\lambda) = \frac{(2m-1)!!}{2^{m+1}}\,\lambda^{-(m+1/2)}\,\sqrt{\pi}, \qquad m = 0, 1, 2, \dots , \tag{C.33}$$

where

$$(2m-1)!! = (2m-1)(2m-3)\dots 3\cdot 1, \qquad (-1)!! = 1, \tag{C.34}$$

Finally, observing that the integrand of (C.30) is even (odd) if n is even (odd), one finds

$$\int_{-\infty}^{+\infty} x^{2m}\,\exp(-\lambda x^2)\,\mathrm{d}x = 2\,I_{2m}(\lambda), \qquad \int_{-\infty}^{+\infty} x^{2m+1}\,\exp(-\lambda x^2)\,\mathrm{d}x = 0. \tag{C.35}$$

The results of this section still hold for a complex λ with $\Re\lambda > 0$.

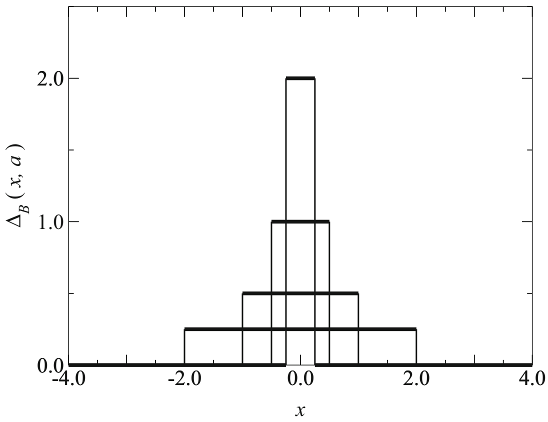

Fig. C.1 Generation of a Dirac δ using a barrier-like function. The width of the peak is equal to a

C.4 Dirac's δ

Consider a function $\Delta_B(x, a)$ defined as follows:

$$\Delta_B = \begin{cases} 1/a & -a/2 \le x \le +a/2 \\ 0 & x < -a/2, \quad x > a/2 \end{cases} \tag{C.36}$$

with $a > 0$.

The above definition yields

$$\lim_{a\to 0} \Delta_B = \begin{cases} 0 & x \ne 0 \\ +\infty & x = 0 \end{cases}, \qquad \int_{-\infty}^{+\infty} \Delta_B(x, a)\,\mathrm{d}x = \frac{1}{a}\int_{-a/2}^{+a/2} \mathrm{d}x = 1. \tag{C.37}$$

As the value of the integral in (C.37) is independent of a, the integral is equal to unity also in the limit $a \to 0$. Figure C.1 shows how the form of Δ_B changes with a: the width of the peak decreases as a decreases, while its height increases so that the area subtending the function remains constant. Note that the procedure depicted above gives a different result if one carries out the integration after calculating the limit. In other terms, the integration and the limit are to be carried out in a specific order (integration first). For a continuous function $f(x)$ the mean-value theorem provides

$$\int_{-\infty}^{+\infty} \Delta_B(x, a)\, f(x)\,\mathrm{d}x = \frac{1}{a}\int_{-a/2}^{+a/2} f(x)\,\mathrm{d}x = f(\bar{x}), \tag{C.38}$$

with $-a/2 < \bar{x} < +a/2$. As a consequence,

$$\lim_{a\to 0}\int_{-\infty}^{+\infty} \Delta_B(x, a)\, f(x)\,\mathrm{d}x = f(0). \tag{C.39}$$

This result is expressed in a more compact form by defining a linear functional $\delta(x)$ (called *Dirac's symbol*) such that

$$\int_{-\infty}^{+\infty} \delta(x)\, f(x)\, \mathrm{d}x = f(0). \tag{C.40}$$

The functional associates the number $f(0)$ to the function $f(x)$. If the reasoning leading to (C.40) is repeated after shifting Δ_B from the origin to another point x_0, one finds the generalization of (C.40)

$$\int_{-\infty}^{+\infty} \delta(x - x_0)\, f(x)\, \mathrm{d}x = f(x_0). \tag{C.41}$$

From (C.41) and (C.16) one obtains

$$\int_{-\infty}^{+\infty} \delta(x - x_0)\, \mathrm{d}x = 1, \qquad \mathcal{F}_x \delta(x - x_0) = \frac{1}{\sqrt{2\pi}} \exp(-\mathrm{i}\, k\, x_0). \tag{C.42}$$

The antitransform (C.17) then reads

$$\delta(x - x_0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp\left[\mathrm{i}\, k\, (x - x_0)\right] \mathrm{d}k, \tag{C.43}$$

that provides an integral representation of the Dirac δ. However, it is important to note that (C.43) has no meaning unless it is used within an integral like, e.g., (C.41). With this provision, one can consider the Dirac δ as the "derivative" of the step function; in fact, after a suitable change in the symbols, one finds that the integral at the right hand side of (C.43) is the derivative with respect to x of the integral at the right hand side of (C.8). More details about the integral representation of the Dirac δ are given in Sect. C.5.

The function $\Delta_B(x, a)$ defined above is an example of generating function of the Dirac δ. Several other examples may be given, as shown below. In all cases, if the generating function $\Delta(x, x_0, a)$ is centered at some point x_0, it is even with respect to x_0 and has the properties $\lim_{a\to 0} \Delta = 0$ if $x \neq x_0$ and $\lim_{a\to 0} \Delta = +\infty$ if $x = x_0$. Consider for instance the Lorentzian function (centered at $x_0 = 0$)

$$\Delta_L = \frac{a/\pi}{a^2 + x^2}, \qquad \int_{-\infty}^{+\infty} \Delta_L\, \mathrm{d}x = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{d}}{\mathrm{d}x} \arctan\left(\frac{x}{a}\right) \mathrm{d}x = 1, \tag{C.44}$$

with $a > 0$. Apart from the limiting case $a \to 0$ the function has only one maximum that occurs at $x = 0$ and equals $1/(a\pi)$. For $x = \pm a$ the function's value halves with respect to the maximum, so $2a$ is conventionally taken as the width of Δ_L. The product $2/\pi$ of the maximum value by the conventional width is independent of a and is of order unity. Finally, for a continuous function $f(x)$ it is

$$\lim_{a\to 0} \int_{-\infty}^{+\infty} \Delta_L(x, a) f(x)\, \mathrm{d}x = f(0). \tag{C.45}$$

Another example of a δ-generating function is the parameterized Gaussian function (centered at $x_0 = 0$)

$$\Delta_G = \frac{\exp(-x^2/a^2)}{a\sqrt{\pi}}, \quad a > 0, \qquad \int_{-\infty}^{+\infty} \Delta_G(x, a)\,\mathrm{d}x = 1 \tag{C.46}$$

(more details about this function and integrals related to it are given in Sects. C.3 and C.8). The function has only one maximum that occurs at $x = 0$ and equals $1/(a\sqrt{\pi})$. For $x = \pm a\sqrt{\log 2} \simeq \pm 0.833\,a$ the function's value halves with respect to the maximum, this yielding a conventional width of $2a\sqrt{\log 2}$. The product $2\sqrt{\log 2}/\sqrt{\pi}$ of the maximum value by the conventional width is independent of a and of order unity. For a continuous function $f(x)$ it is

$$\lim_{a\to 0} \int_{-\infty}^{+\infty} \Delta_G(x, a) f(x)\,\mathrm{d}x = f(0). \tag{C.47}$$

A final example of a δ-generating function is the negative derivative of the Fermi-Dirac statistics (centered at $x_0 = 0$)

$$\Delta_F = -\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{\exp(x/a) + 1} = \frac{\exp(x/a)}{a\left[\exp(x/a) + 1\right]^2}, \qquad a > 0, \tag{C.48}$$

$$\int_{-\infty}^{+\infty} \Delta_F(x, a)\,\mathrm{d}x = \int_{+\infty}^{-\infty} \frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{\exp(x/a) + 1}\,\mathrm{d}x = 1. \tag{C.49}$$

(more details about this function and integrals related to it are given in Sect. C.13). The function has only one maximum that occurs at $x = 0$ and equals $1/(4a)$. For $x = \pm a \log(3+\sqrt{8}) \simeq \pm 1.76\,a$ the function's value halves with respect to the maximum, this yielding a conventional width of $2a \log(3+\sqrt{8})$. The product $(1/2)\,\log(3+\sqrt{8})$ of the maximum value by the conventional width is independent of a and of order unity. For a continuous function $f(x)$ it is

$$\lim_{a\to 0} \int_{-\infty}^{+\infty} \Delta_F(x, a) f(x)\,\mathrm{d}x = f(0). \tag{C.50}$$

The δ-generating functions Δ vanish for $x \to \pm\infty$, otherwise they would not be integrable from $-\infty$ to $+\infty$. Assuming that Δ is differentiable with respect to x yields, after integrating by parts,

$$\int_{-\infty}^{+\infty} f(x)\,\frac{\mathrm{d}\Delta(x, a)}{\mathrm{d}x}\,\mathrm{d}x = [\Delta(x, a)\, f(x)]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \Delta(x, a)\,\frac{\mathrm{d}f}{\mathrm{d}x}\,\mathrm{d}x, \tag{C.51}$$

with f a differentiable function. In (C.51) the integrated part is zero because Δ vanishes at infinity. Taking the limit $a \to 0$ at both sides of (C.51) and using (C.40) yields

$$\int_{-\infty}^{+\infty} f(x)\,\frac{\mathrm{d}\delta(x)}{\mathrm{d}x}\,\mathrm{d}x = -\int_{-\infty}^{+\infty} \delta(x)\,\frac{\mathrm{d}f}{\mathrm{d}x}\,\mathrm{d}x = -f'(0), \tag{C.52}$$

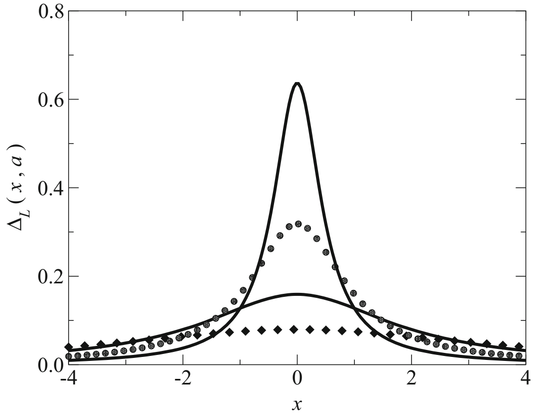

Fig. C.2 Generation of a Dirac δ using a Lorentzian function. The width of the peak is proportional to a

which is used as the definition of the derivative of δ. Such a definition generalizes to

$$\int_{-\infty}^{+\infty} f(x)\,\frac{\mathrm{d}^n\delta(x)}{\mathrm{d}x^n}\,\mathrm{d}x = (-1)^n\, f^{(n)}(0). \tag{C.53}$$

C.5 Some Properties of Dirac's δ

An integral representation of δ is derived from (C.18) after rearranging it as

$$f(x) = \int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty}\frac{\exp\left[\mathrm{i}\,k\,(x-\xi)\right]}{2\,\pi}\,\mathrm{d}k\right] f(\xi)\,\mathrm{d}\xi \tag{C.54}$$

and comparing with (C.41):

$$\delta(\xi - x) = \int_{-\infty}^{+\infty}\frac{\exp\left[\mathrm{i}\,k\,(x-\xi)\right]}{2\,\pi}\,\mathrm{d}k. \tag{C.55}$$

Replacing k with $-k$ in (C.55) shows that δ is even with respect to its argument, $\delta(x-\xi) = \delta(\xi - x)$. Also, comparing (C.55) with (C.16) shows that $\delta(\xi - x)$ is the Fourier transform of $\exp(\mathrm{i}\,k\,x)/\sqrt{2\,\pi}$. The generalization of (C.55) to more than one dimension is immediate; e.g., the three-dimensional case reads

$$\delta(\mathbf{g} - \mathbf{x}) = \iiint_{-\infty}^{+\infty}\frac{\exp\left[\mathrm{i}\,\mathbf{k}\cdot(\mathbf{x}-\mathbf{g})\right]}{(2\,\pi)^3}\,\mathrm{d}^3k. \tag{C.56}$$

The discrete-case analogue of (C.56) is given by (C.117, C.121), where the generalization of the Kronecker symbol is given. Note that the latter is dimensionless, whereas the units of Dirac's δ depend on its argument: by way of example, the integral $\int_{-\infty}^{+\infty}\delta(\xi - x)\,\mathrm{d}\xi = 1$ shows that the units of $\delta(\xi - x)$ are the inverse of those of

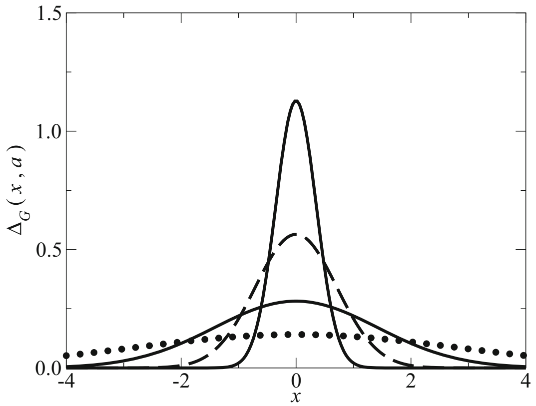

Fig. C.3 Generation of a Dirac δ using a parameterized Gaussian function. The width of the peak is proportional to a

$\mathrm{d}\xi$; similarly, the integral $\iiint_{-\infty}^{+\infty} \delta(\mathbf{g} - \mathbf{x})\, \mathrm{d}^3 g = 1$ shows that the units of $\delta(\mathbf{g} - \mathbf{x})$ are the inverse of those of $\mathrm{d}^3 g$, and so on.

A generalization of Dirac's δ is found by replacing $\delta(x)$ with $\delta[q(x)]$, with $q(x)$ a function having one or more zeros. Let x_1 be a simple zero of q, namely, $q'(x_1) \neq 0$, and consider the contribution of it to the integral $\int_{-\infty}^{+\infty} \delta[q(x)]\, \mathrm{d}x$. Observing that in a finite neighborhood I_1 of x_1 there are no other zeros, one can determine such a contribution by replacing $q(x)$ with $q'(x_1)\,(x - x_1)$; in this way, to bring the calculation back to the standard form one may provisionally scale the differential $\mathrm{d}x$ by $1/q'(x_1)$. However, if the scaling factor were negative, the evenness of δ would be violated; thus, the correct scaling factor is $|q'(x_1)|$, and

$$\int_{I_1} \delta[q(x)]\, f(x)\, \mathrm{d}x = \frac{1}{|q'(x_1)|}\, f(x_1). \tag{C.57}$$

If q has n simple zeros, from (C.57) it follows

$$\int_{-\infty}^{+\infty} \delta[q(x)]\, f(x)\, \mathrm{d}x = \frac{1}{|q'(x_1)|}\, f(x_1) + \ldots + \frac{1}{|q'(x_n)|}\, f(x_n). \tag{C.58}$$

C.6 Moments Expansion

For a given function $f(k)$ consider the integral

$$M_n = \int_{-\infty}^{+\infty} k^n f(k)\, \mathrm{d}k, \qquad n = 0, 1, \ldots \tag{C.59}$$

It is assumed that the integral converges for any n. This implies that f vanishes at infinity with a strength larger than any power. As the present considerations apply to a distribution function, the vanishing of f is typically of the exponential type. The quantity M_n is called *moment of order n* of function f. Thanks to its properties, f can be Fourier transformed; let

$$g(y) = \mathcal{F} f = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(k)\, \exp(-\mathrm{i}\, y\, k)\, \mathrm{d}k. \tag{C.60}$$

Using the Taylor expansion $\exp(-\mathrm{i}\, y\, k) = \sum_{n=0}^{\infty} (-\mathrm{i}\, y\, k)^n / n!$ yields

$$g(y) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{(-\mathrm{i})^n M_n}{\sqrt{2\pi}} y^n. \tag{C.61}$$

The latter is the Taylor expansion of g around the origin; it follows

$$\frac{(-\mathrm{i})^n M_n}{\sqrt{2\pi}} = \left(\frac{\mathrm{d}^n g}{\mathrm{d}y^n}\right)_0. \tag{C.62}$$

The above analysis shows that, if the moments M_n of $f(k)$ are known, from them one constructs the Fourier transform $g(y) = \mathcal{F} f$ by means of a Taylor series. Then, one recovers the original function from the inverse transform $f(k) = \mathcal{F}^{-1} g$. In conclusion, the knowledge of the set of moments of f is equivalent to the knowledge of f. The result holds true also in the multi-dimensional case $f = f(\mathbf{k})$, where

$$M_{l+m+n} = \iiint_{-\infty}^{+\infty} k_1^l\, k_2^m\, k_3^n\, f(\mathbf{k})\, \mathrm{d}^3 k, \qquad l, m, n = 0, 1, \ldots \tag{C.63}$$

is the moment of order $l + m + n$ of f.

If only the lower-order moments are used, then the Taylor series for the Fourier transform is truncated and provides an approximation $\tilde{g}$ for g. As a consequence of this approximation, the inverse transform $\tilde{f} = \mathcal{F}^{-1} \tilde{g}$ provides an approximate form of the original function f.

An extension of the above concepts is obtained by replacing the monomial expression $k_1^l\, k_2^m\, k_3^n$ with a function $\alpha(\mathbf{k})$, that can be expressed by a polynomial interpolation. In this case, in fact, the integral of $\alpha(\mathbf{k})\, f(\mathbf{k})$ is a combination of moments of f. A further generalization consists in considering f, α, or both, as functions of other variables besides $\mathbf{k}$:

$$M_\alpha(\mathbf{r}, t) = \iiint_{-\infty}^{+\infty} \alpha(\mathbf{r}, \mathbf{k}, t)\, f(\mathbf{r}, \mathbf{k}, t)\, \mathrm{d}^3 k. \tag{C.64}$$

If $f(\mathbf{r}, \mathbf{k}, t)$ is the solution of a differential equation generated by an operator $\mathcal{A}$, say, $\mathcal{A} f = 0$, one can derive a set of moments from such an equation by selecting different forms of α:

$$\iiint_{-\infty}^{+\infty} \alpha\, \mathcal{A} f\, \mathrm{d}^3 k = 0. \tag{C.65}$$

Each moment depends on the other variables $\mathbf{r}, t$. If operator $\mathcal{A}$ contains the derivatives with respect to $\mathbf{r}$, t, or both, then the moment of $\mathcal{A} f = 0$ is a differential equation in $\mathbf{r}$, t, or both.

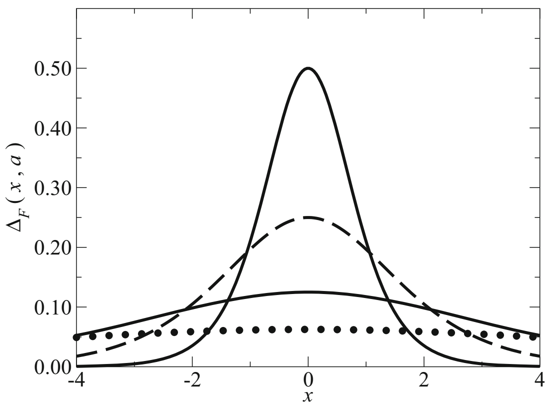

Fig. C.4 Generation of a Dirac δ using a Fermi-Dirac statistics. The width of the peak is proportional to a

C.7 Error Function

The *error function* and the *complementary error function* are defined, respectively, as

$$\mathrm{erf}\,(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp\,(-\xi^2)\,\mathrm{d}\xi, \qquad \mathrm{erfc}\,(x) = 1 - \mathrm{erf}\,(x). \tag{C.66}$$

From the definitions (C.66) and from the Gauss integral (C.23) the following properties are derived:

$$\frac{\mathrm{d}}{\mathrm{d}x}\,\mathrm{erf}\,(x) = \frac{2}{\sqrt{\pi}} \exp\,(-x^2), \qquad \mathrm{erf}\,(-x) = -\,\mathrm{erf}\,(x), \tag{C.67}$$

$$\mathrm{erf}\,(-\infty) = -1, \qquad \mathrm{erf}\,(0) = 0, \qquad \mathrm{erf}\,(+\infty) = 1, \tag{C.68}$$

$$\mathrm{erfc}\,(-\infty) = 2, \qquad \mathrm{erfc}\,(0) = 1, \qquad \mathrm{erfc}\,(+\infty) = 0. \tag{C.69}$$

Integrating by parts yields

$$\int_0^x \mathrm{erfc}\,(\xi)\,\mathrm{d}\xi = x\,\mathrm{erfc}\,(x) + \frac{1}{\sqrt{\pi}}\left[1 - \exp\,(-x^2)\right]. \tag{C.70}$$

Applying the de l'Hôpital rule shows that the first term at the right hand side of (C.70) vanishes for $x \to +\infty$. It follows

$$\int_0^{+\infty} \mathrm{erfc}\,(x)\,\mathrm{d}x = \frac{1}{\sqrt{\pi}}. \tag{C.71}$$

Still applying the de l'Hôpital rule shows that

$$\lim_{x\to 0} \frac{\mathrm{erf}\,(x)}{x} = \frac{2}{\sqrt{\pi}}, \qquad \lim_{x\to+\infty} \frac{\mathrm{erfc}\,(x)}{\exp\,(-x^2)} = \lim_{x\to+\infty} \frac{1/\sqrt{\pi}}{x}, \tag{C.72}$$

whence

$$\operatorname{erf}(x) \simeq \frac{2}{\sqrt{\pi}}\, x \quad \text{for} \quad |x| \ll 1, \qquad \operatorname{erfc}(x) \simeq \frac{1}{\sqrt{\pi}}\, \frac{\exp(-x^2)}{x} \quad \text{for} \quad x \gg 1. \tag{C.73}$$

Other applications of the integration by parts yield

$$Y = \int_0^x \xi\, \operatorname{erfc}(\xi)\, \mathrm{d}\xi = x^2\, \operatorname{erfc}(x) - Y - \frac{1}{\sqrt{\pi}} \int_0^x \xi \left[\frac{\mathrm{d}}{\mathrm{d}\xi} \exp(-\xi^2)\right] \mathrm{d}\xi =$$

$$= \frac{1}{2}\, x^2\, \operatorname{erfc}(x) + \frac{1}{4}\, \operatorname{erf}(x) - \frac{1}{2\sqrt{\pi}}\, x\, \exp(-x^2). \tag{C.74}$$

C.8 Parametrized Gaussian Function

The relations introduced in Sects. C.3 and C.7 are useful for investigating the properties of function

$$\Delta(x-\xi, a) = \frac{\exp[-(x-\xi)^2/(4\,a)]}{\sqrt{4\pi\, a}}, \qquad a > 0. \tag{C.75}$$

The behavior of Δ in the limit $a \to 0$ depends on the argument $x - \xi$, namely

$$\lim_{a\to 0} \Delta(x-\xi, a) = \begin{cases} 0 & \xi \neq x \\ +\infty & \xi = x \end{cases} \tag{C.76}$$

In contrast, its integral over ξ is independent of x and a. In fact, using (C.23) after letting $\mu = (x-\xi)/\sqrt{4a}$ yields

$$\int_{-\infty}^{+\infty} \Delta(x-\xi, a)\, \mathrm{d}\xi = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp(-\mu^2)\, \mathrm{d}\mu = 1. \tag{C.77}$$

Adopting the same variable change leading to (C.77) and using (C.23, C.66) yields

$$\int_{-\infty}^{0} \Delta(x-\xi, a)\, \mathrm{d}\xi = \frac{1}{2}\, \operatorname{erfc}\left(\frac{x}{\sqrt{4a}}\right). \tag{C.78}$$

The relations (C.77, C.78) hold also in the limit for $a \to 0$, provided the limit is calculated *after* the integration. This property is typical of the functions that generate the Dirac δ (Sect. C.4). In fact it can be shown that for a continuous function $g(x)$ the following holds:

$$\lim_{a\to 0} \int_{-\infty}^{+\infty} g(\xi)\, \Delta(x-\xi, a)\, \mathrm{d}\xi = g(x). \tag{C.79}$$

Other examples of δ-generating functions are given in Sect. C.4. This section is concluded by showing that $\Delta(x-\xi, a)$ admits an integral representation of the form

$$\Delta(x-\xi, a) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \exp\left[\mathrm{i}k(x-\xi) - ak^2\right] \mathrm{d}k. \tag{C.80}$$

To prove (C.80) one recasts the argument of the exponential by means of the identity

$$\mathrm{i}k(x-\xi) - ak^2 = -\frac{(x-\xi)^2}{4a} - a\left[k - \frac{\mathrm{i}(x-\xi)}{2a}\right]^2, \tag{C.81}$$

and uses (C.23) with $\sqrt{a}\,[k - \mathrm{i}(x-\xi)/(2a)]$ as the integration variable. It is interesting to note in passing that letting $\xi = 0$, $a = \sigma^2/2$ in (C.80) yields

$$\exp\left[-x^2/(2\,\sigma^2)\right] = \frac{\sigma}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \exp\left(-\sigma^2 k^2/2\right)\,\exp\left(\mathrm{i}\,k\,x\right)\mathrm{d}k, \tag{C.82}$$

namely, the Gaussian function is the Fourier transform of itself.

C.9 Euler's Beta Function

The function defined by the integral

$$B(\lambda,\ \mu) = \int_0^1 x^{\lambda-1}\,(1-x)^{\mu-1}\,\mathrm{d}x, \tag{C.83}$$

with λ, μ complex numbers such that $\Re(\lambda) > 0$, $\Re(\mu) > 0$, is called *Euler's Beta function* or *Euler's integral of the first kind* [65]. Letting $x = y/(y+1)$ and replacing y with x gives (C.83) the equivalent form

$$B(\lambda,\ \mu) = \int_0^{+\infty} x^{\lambda-1}\,(1+x)^{-(\lambda+\mu)}\,\mathrm{d}x. \tag{C.84}$$

Limiting the variables' range to $0 < \Re(\lambda), \Re(\mu) < 1$ and letting

$$\mu = 1-\lambda, \qquad T_0(\lambda) = B(\lambda, 1-\lambda) \tag{C.85}$$

yields

$$T_0(\lambda) = \int_0^{+\infty} \frac{x^{\lambda-1}}{1+x}\,\mathrm{d}x = \frac{\pi}{\sin(\lambda\pi)}. \tag{C.86}$$

The last equality is demonstrated by applying Cauchy's residue theorem [114, Sect. 64] to the function $f(z) = z^{\lambda-1}/(1+z)$, with z complex, that over the real axis reduces to the integrand of (C.86). The relation (C.86) can be exploited for calculating other integrals. For instance, for λ real one lets $\lambda = 1/(2\mu)$, $x = y^{2\mu}$ to find

$$\int_0^{+\infty} \frac{1}{1+y^{2\mu}}\,\mathrm{d}y = \frac{\pi/(2\mu)}{\sin\left[\pi/(2\mu)\right]}, \qquad \mu > \frac{1}{2}. \tag{C.87}$$

C.10 Euler's Gamma Function

The function defined by the integral

$$\Gamma(\lambda) = \int_0^{+\infty} x^{\lambda-1} \exp(-x)\,\mathrm{d}x, \tag{C.88}$$

with λ a complex number such that $\Re(\lambda) > 0$, is called *Euler's Gamma function* or *Euler's integral of the second kind* [33, Sect. 1.3].[5] The negative of its derivative $\Gamma' = \mathrm{d}\Gamma/\mathrm{d}\lambda$ calculated for $\lambda = 1$ is called *Euler's constant*, $\gamma = -\Gamma'(1) = \int_0^{+\infty} \exp(-x) \log(x)\,\mathrm{d}x \simeq 0.5772$. From (C.88) one finds $\Gamma(1) = 1$ and, after integrating by parts,

$$\Gamma(\lambda + 1) = \lambda\, \Gamma(\lambda). \tag{C.89}$$

If $\lambda = n = 1, 2, \ldots$ (C.89) yields

$$\Gamma(n + 1) = n\, \Gamma(n) = n(n - 1)\, \Gamma(n - 1) = \ldots = n!. \tag{C.90}$$

The definition of Γ is extended by analytic continuation to the complex plane with the exception of the points $\lambda = 0, -1, -2, \ldots, -n, \ldots$. At each negative integer $-n$, the function Γ has a simple pole with a residue equal to $(-1)^n/n!$ [65], namely,

$$\lim_{\lambda \to -n} (\lambda + n)\, \Gamma(\lambda) = \frac{(-1)^n}{n!}, \qquad n = 0, 1, 2 \ldots \tag{C.91}$$

A straightforward calculation shows that the beta and gamma functions are connected by the relation [65]

$$\Gamma(\lambda)\, \Gamma(\mu) = \Gamma(\lambda + \mu)\, B(\lambda, \mu). \tag{C.92}$$

Thanks to (C.92) one extends the definition of B to the complex plane with the exception of the points $\lambda, \mu, \lambda + \mu = 0, -1, -2, \ldots, -n, \ldots$. Moreover, limiting the variables' range to $0 < \Re(\lambda), \Re(\mu) < 1$ and letting $\mu = 1 - \lambda$ so that $\Gamma(\lambda + \mu) = \Gamma(1) = 1$, from (C.86) one finds

$$\Gamma(\lambda)\, \Gamma(1 - \lambda) = \int_0^{+\infty} \frac{x^{\lambda-1}}{1 + x}\,\mathrm{d}x = T_0(\lambda), \qquad 0 < \Re(\lambda) < 1. \tag{C.93}$$

For $\lambda = 1/2$ (C.93) yields

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi} \tag{C.94}$$

---

[5] As remarked in [33], Legendre's notation $\Gamma(\lambda)$ is unfortunate because the argument that appears at the right hand side of the definition is $\lambda - 1$. Gauss used the notation $\Pi(\lambda - 1)$ for the left hand side of C.88.

whence, thanks to (C.89),

$$\Gamma\left(\frac{3}{2}\right)=\frac{1}{2}\,\Gamma\left(\frac{1}{2}\right)=\frac{1}{2}\sqrt{\pi},\quad \Gamma\left(\frac{5}{2}\right)=\frac{3}{2}\,\Gamma\left(\frac{3}{2}\right)=\frac{3}{4}\sqrt{\pi},\quad \ldots \tag{C.95}$$

Iterating (C.95) and comparing with (C.33) shows that $\Gamma(m+1/2) = 2\,I_{2m}(1)$, $m = 0, 1, 2, \ldots$

C.11 Gamma Function's Asymptotic Behavior

Euler's Gamma function introduced in Sect. C.10, considered for real values of λ, lends itself to a significant application of the asymptotic analysis. Specifically, one seeks another function $f(\lambda)$, expressible through elementary functions, such that $\lim_{\lambda\to\infty}[\Gamma(\lambda+1)/f(\lambda)] = 1$. The asymptotic analysis applied to the Γ function shows that [26]

$$\lim_{\lambda\to\infty}\frac{\Gamma(\lambda+1)}{\lambda^{\lambda+1/2}\exp(-\lambda)}=\sqrt{2\pi}, \tag{C.96}$$

namely, the function sought is $f(\lambda) = \sqrt{2\pi}\,\lambda^{\lambda+1/2}\exp(-\lambda)$. Equation (C.96) is called *Stirling's formula*. Remembering (C.90) one has $\Gamma(\lambda+1) = \Gamma(n+1) = n!$ when λ is a natural number. From (C.96) it follows

$$n! \simeq \sqrt{2\pi}\,n^{n+1/2}\ \exp(-n) = \sqrt{2\pi\,n}\ (n/\mathrm{e})^n\,, \tag{C.97}$$

that provides an approximation to the factorial for $n \gg 1$. Letting by way of example $n = 10$, the rounded value of the right hand side of (C.97) turns out to be 3 598 696, that differs from $10! = 3\,628\,800$ by less than 1%.

The asymptotic value of the derivative of $\log\Gamma$ is also of interest, for instance when determining the equilibrium distribution of particles in statistical mechanics (Sects. 6.4, 15.8.1,15.8.2). Using (C.96) one finds

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\log\Gamma(\lambda+1)\simeq\frac{1}{2\,\lambda}+\log\lambda\simeq\log\lambda,\qquad \lambda\gg 1. \tag{C.98}$$

C.12 Integrals Related to the Harmonic Oscillator

Consider the integral

$$I(s)=\int_0^1\frac{\mathrm{d}\xi}{\sqrt{1-\xi^s}}, \tag{C.99}$$

where s is a real parameter, $s > 0$. Letting $u = \xi^s$ one finds $1/\sqrt{1-\xi^s} = (1-u)^{1/2-1}$, $\mathrm{d}\xi = u^{1/s-1}\,\mathrm{d}u/s$ whence, using (C.83, C.92, C.94),

$$I(s)=\frac{1}{s}\,B(1/s,1/2)=\frac{\sqrt{\pi}}{s}\,\frac{\Gamma(1/s)}{\Gamma(1/s+1/2)}. \tag{C.100}$$

By way of example $I(2) = \pi/2$, which can also be derived directly from (C.99). When $s \to \infty$ one can use (C.91) with $n = 0$. It follows

$$\lim_{s\to\infty} I(s) = 1. \tag{C.101}$$

Now consider the integral

$$J(s) = \int_0^1 \frac{d\xi}{\sqrt{1/\xi^s - 1}}, \tag{C.102}$$

still with $s > 0$. The same procedure used for calculating $I(s)$ yields

$$J(s) = \frac{1}{s}\, B(1/s + 1/2, 1/2) = \frac{\sqrt{\pi}}{s}\, \frac{\Gamma(1/s + 1/2)}{\Gamma(1/s + 1)} = \frac{\pi}{s}\, \frac{1}{I(s)}, \tag{C.103}$$

and $\lim_{s\to\infty} J(s) = 0$. By way of example $J(1) = \pi/2$, which can also be derived directly from (C.102). The integrals (C.100, C.103) appear in the theory of the harmonic oscillator (Sect. 3.3 and Problems 3.1, 3.2).

C.13 Fermi Integrals

The *Fermi integral* of order α is defined as

$$\Phi_\alpha(\xi) = \frac{1}{\Gamma(\alpha + 1)} \int_0^\infty \frac{x^\alpha}{1 + \exp(x - \xi)}\, dx, \qquad \alpha > -1, \tag{C.104}$$

where Γ is defined by (C.88) and α is a real parameter. The constraint $\alpha > -1$ guarantees the convergence of the integral. If $-\xi \gg 1$ one has $\exp(x - \xi) \geq \exp(-\xi) \gg 1$ and, from (C.88),

$$\Phi_\alpha(\xi) \simeq \frac{\exp(\xi)}{\Gamma(\alpha + 1)} \int_0^\infty x^\alpha \exp(-x)\, dx = \exp(\xi), \qquad \xi \gg -1. \tag{C.105}$$

A relation between Fermi integral of different order is found by considering, for some $\alpha > 0$, the integral of order $\alpha - 1$:

$$\frac{1}{\Gamma(\alpha)} \int_0^\infty \frac{x^{\alpha-1}}{1 + \exp(x - \xi)}\, dx = \frac{1}{\alpha\, \Gamma(\alpha)} \int_0^\infty \frac{x^\alpha \exp(x - \xi)}{[1 + \exp(x - \xi)]^2}\, dx, \tag{C.106}$$

where the right hand side is derived through an integration by parts. Observing that $\alpha\, \Gamma(\alpha) = \Gamma(\alpha + 1)$ and using again (C.104) shows that the right hand side of (C.106) is equal to $d\Phi_\alpha/d\xi$. Then,

$$\frac{d\Phi_\alpha}{d\xi} = \Phi_{\alpha-1}, \qquad \frac{d \log \Phi_\alpha}{d\xi} = \frac{\Phi_{\alpha-1}}{\Phi_\alpha}. \tag{C.107}$$

The Fermi integrals are positive by construction; from the first relation in (C.107) it then follows that the Fermi integrals are monotonically-increasing functions of the argument ξ. The Fermi integral of order 0 is expressed in terms of elementary functions,

$$\Phi_0 = \log\left[\exp(\xi) + 1\right]. \tag{C.108}$$

Approximations for the Fermi integrals are found, e.g., in [6, Appendix C]. In the applications to the semiconductor theory the Fermi integrals of small half-integer order (1/2, 3/2) are the most important ones (Sects. 18.2, 19.6.4). Remembering (C.94, C.95), they read

$$\Phi_{1/2}(\xi) = \int_0^\infty \frac{2\,x^{1/2}/\sqrt{\pi}}{1+\exp(x-\xi)}\,\mathrm{d}x, \quad \Phi_{3/2}(\xi) = \int_0^\infty \frac{(4/3)\,x^{3/2}/\sqrt{\pi}}{1+\exp(x-\xi)}\,\mathrm{d}x. \tag{C.109}$$

C.14 Hölder's Inequality

Hölder's inequality states that for any pair of real constants $b, c > 1$ such that $1/b + 1/c = 1$ it is

$$\int_\eta |F\,G|\,\mathrm{d}x \le \left(\int_\eta |F|^b\,\mathrm{d}x\right)^{1/b} \left(\int_\eta |G|^c\,\mathrm{d}x\right)^{1/c}, \tag{C.110}$$

where F, G are any complex functions defined over the real interval η and such that the integrals in (C.110) converge. The inequality is proven starting from the function $\varphi(r) = r^b - b\,r + b - 1$, $r > 0$, $b > 1$, whose first derivative is $\varphi'(r) = b\,r^{b-1} - b$ and the second one $\varphi'' = b\,(b-1)\,r^{b-2}$. As a consequence, for $r > 0$ the function has only one minimum, located at $r = 1$. The inequality $r^b + b \ge b\,r + 1$ then holds, whence

$$\frac{r^{b-1}}{b} + \frac{1}{c\,r} \ge 1, \quad c = \frac{b}{b-1} > 1. \tag{C.111}$$

Let $F_1(x)$ and $G_1(x)$ be any two complex functions defined over η and fulfilling the normalization condition

$$\int_\eta |F_1|^b\,\mathrm{d}x = \int_\eta |G_1|^c\,\mathrm{d}x = 1. \tag{C.112}$$

Letting $r^{b-1} = |F_1|^{b-1}/|G_1|$ and replacing in (C.111) yields

$$\frac{|F_1|^b}{b} + \frac{|G_1|^c}{c} - |F_1\,G_1| \ge 0, \qquad \frac{1}{b} + \frac{1}{c} = 1. \tag{C.113}$$

Since the function at the left hand side of (C.113) is non negative, its integral is non negative as well. Integrating (C.113) over η and using the normalization condition (C.112) yields

$$\int_\eta |F_1\, G_1|\, \mathrm{d}x \le \frac{1}{b} + \frac{1}{c} = 1. \tag{C.114}$$

On the other hand the normalization condition also yields

$$\left(\int_\eta |F_1|^b\, \mathrm{d}x\right)^{1/b} = \left(\int_\eta |G_1|^c\, \mathrm{d}x\right)^{1/c} = 1, \tag{C.115}$$

whence

$$\int_\eta |F_1 G_1|\, \mathrm{d}x \le \left(\int_\eta |F_1|^b\, \mathrm{d}x\right)^{1/b} \left(\int_\eta |G_1|^c\, \mathrm{d}x\right)^{1/c}. \tag{C.116}$$

As (C.116) is homogeneous, it still holds after replacing F_1, G_1 with $F = \lambda\, F_1$ and $G = \mu\, G_1$, where λ, μ are arbitrary positive real numbers. This proves Hölder's inequality (C.110).

C.15 Integrals Related to the Electromagnetic Modes

In several applications (e.g., calculations related to the modes of the electromagnetic field, Sect. 5.5) one must evaluate integrals of the form

$$Y = \int_V \exp\left[\mathrm{i}\,(\mathbf{k} \pm \mathbf{k}') \cdot \mathbf{r}\right] \mathrm{d}^3 r, \tag{C.117}$$

where $\mathbf{k} = \mathbf{k}(n_1, n_2, n_3)$ is given by

$$\mathbf{k} = n_1\, \frac{2\,\pi}{d_1}\, \mathbf{i}_1 + n_2\, \frac{2\,\pi}{d_2}\, \mathbf{i}_2 + n_3\, \frac{2\,\pi}{d_3}\, \mathbf{i}_3, \qquad n_i = 0, \pm 1, \pm 2, \ldots, \tag{C.118}$$

$\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3$ being the unit vectors parallel to the coordinate axes. The integration domain in (C.117) is a box whose sides d_1, d_2, d_3 are aligned with the axes and start from the origin (Fig. 5.1). The volume of the box is $V = d_1\, d_2\, d_3$. As $(\mathbf{k} \pm \mathbf{k}') \cdot \mathbf{r} = (k_1 \pm k_1')\, x_1 + (k_2 \pm k_2')\, x_2 + (k_3 \pm k_3')\, x_3$, where the upper (lower) signs hold together, the integral becomes $Y = Y_1\, Y_2\, Y_3$, with

$$Y_i = \int_0^{d_i} \exp\left[\mathrm{i}\,(k_i \pm k_i')\, x_i\right] \mathrm{d}x_i = \frac{\exp\left[\mathrm{i}\,(k_i \pm k_i')\, d_i\right] - 1}{\mathrm{i}\,(k_i \pm k_i')}. \tag{C.119}$$

Letting $\theta_i = (k_i \pm k_i')\, d_i/2 = \pi\,(n_i \pm n_i')$, (C.119) becomes

$$Y_i = d_i\, \exp(\mathrm{i}\,\theta_i)\, \frac{\exp(\mathrm{i}\,\theta_i) - \exp(-\mathrm{i}\,\theta_i)}{2\,\mathrm{i}\,\theta_i} = d_i\, \exp(\mathrm{i}\,\theta_i)\, \frac{\sin\theta_i}{\theta_i}. \tag{C.120}$$

It follows that $Y_i = 0$ if $n_i \pm n_i' \neq 0$, while $Y_i = d_i$ if $n_i \pm n_i' = 0$. Combining the three integrals shows that it is $Y = 0$ if $\mathbf{k} \pm \mathbf{k}' \neq 0$, while it is $Y = V$ if $\mathbf{k} \pm \mathbf{k}' = 0$. The result is recast in a compact form by means of the three-dimensional extension of the Kronecker symbol (A.18):

$$Y = V\,\delta[\mathbf{k} \pm \mathbf{k}', 0] = V\,\delta[\mathbf{k} \pm \mathbf{k}'], \tag{C.121}$$

where the last form is obtained by dropping the zero for the sake of conciseness. Compare (C.117, C.121) with (C.56) and the comments therein.

C.16 Riemann's Zeta Function

The function defined by

$$\zeta(\lambda, a) = \sum_{k=1}^{\infty} \frac{1}{(k+a)^{\lambda}}, \tag{C.122}$$

where λ is a complex number with $\Re(\lambda) > 1$ and $a \geq 0$ is real, is called *Riemann's Zeta function*. It can be represented in integral form by combining it with the Gamma function (C.88): letting $x = (k+a)\,y$ in the latter, then replacing y back with x, yields

$$\Gamma(\lambda) = (k+a)^{\lambda} \int_0^{+\infty} x^{\lambda-1} \exp\left[-(k+a)\,x\right] \mathrm{d}x. \tag{C.123}$$

Dividing (C.123) by $(k+a)^{\lambda}$, letting $k = 1, 2, \ldots$, and adding over k provides

$$\Gamma(\lambda) \sum_{k=1}^{\infty} \frac{1}{(k+a)^{\lambda}} = \int_0^{+\infty} x^{\lambda-1} \exp(-ax) \left[\sum_{k=1}^{\infty} \exp(-kx)\right] \mathrm{d}x, \tag{C.124}$$

where $\sum_{k=1}^{\infty} \exp(-k\,x) = \exp(-x)\left[1 + \exp(-x) + \exp(-2\,x) + \ldots\right] = 1/[\exp(x) - 1]$, so that from (C.122),

$$\zeta(\lambda, a) = \frac{1}{\Gamma(\lambda)} \int_0^{+\infty} \frac{x^{\lambda-1}}{\exp(x) - 1} \exp(-a\,x)\,\mathrm{d}x, \qquad \Re(\lambda) > 1. \tag{C.125}$$

Remembering (C.89) one finds that (C.125) fulfills the recursive relation

$$\frac{\partial}{\partial a} \zeta(\lambda, a) = -\lambda\, \zeta(\lambda + 1, a). \tag{C.126}$$

Also, letting $a = 0$ and $\lambda = 2\,m$, with $m = 1, 2, \ldots$ transforms (C.125) into

$$\int_0^{+\infty} \frac{x^{2\,m-1}}{\exp(x) - 1}\,\mathrm{d}x = \Gamma(2\,m)\,\zeta(2\,m, 0) = \frac{(2\,\pi)^{2\,m}}{4\,m}\,|B_{2m}|, \tag{C.127}$$

with $B_{2m} = (-1)^{m+1}\,|B_{2m}|$, $m \geq 1$ the *Bernoulli number*[6] of order $2\,m$ [44]. Thanks to (C.127) one calculates integrals used in different applications. For instance, letting $m = 2$ and using $B_4 = -1/30$

$$\int_0^{+\infty} \frac{x^3}{\exp(x) - 1}\,\mathrm{d}x = \frac{1}{15}\pi^4, \tag{C.128}$$

that is used in (15.78) to calculate the Lagrangian multiplier in the equilibrium statistics for photons. From (C.125) one derives another important class of integrals; in fact, replacing x with $2\,x$ in the denominator of (C.125) yields

$$\int_0^{+\infty} \frac{x^{\lambda-1}}{\exp(2\,x) - 1}\,\exp(-a\,x)\,\mathrm{d}x = 2^{-\lambda}\,\Gamma(\lambda)\,\zeta(\lambda, a/2), \qquad \Re(\lambda) > 1 \tag{C.129}$$

whence, using the identity $2/[\exp(2\,x) - 1] = 1/[\exp(x) - 1] - 1/[\exp(x) + 1]$ within (C.125), (C.129) provides

$$\int_0^{+\infty} \frac{x^{\lambda-1}}{\exp(x) + 1}\,\exp(-a\,x)\,\mathrm{d}x = \Gamma(\lambda)\,\left[\zeta(\lambda, a) - 2^{1-\lambda}\,\zeta(\lambda, a/2)\right]. \tag{C.130}$$

Letting $a = 0$ and $\lambda = 2\,m$, $m = 1, 2, \ldots$ in the latter, and using (C.127), transforms (C.130) into

$$\int_0^{+\infty} \frac{x^{2\,m-1}}{\exp(x) + 1}\,\mathrm{d}x = \frac{\pi^{2\,m}}{2\,m}\,\left(2^{2\,m-1} - 1\right)\,|B_{2m}|. \tag{C.131}$$

For instance, for $m = 1$ and $m = 2$, (C.131) provides

$$\int_0^{+\infty} \frac{x}{\exp(x) + 1}\,\mathrm{d}x = \frac{1}{12}\,\pi^2, \qquad \int_0^{+\infty} \frac{x^3}{\exp(x) + 1}\,\mathrm{d}x = \frac{7}{120}\,\pi^4. \tag{C.132}$$

[6] The Bernoulli numbers are defined by the series expansion $x/[\exp(x) - 1] = \sum_0^\infty B_n\,x^n/n!$, with $|x| < 2\,\pi$. It is $B_0 = 1$, $B_1 = -1/2$, $B_2 = 1/6$, $B_4 = -1/30$. Apart from B_1, all Bernoulli numbers of odd index vanish.

Appendix D
Tables

Table D.1 Fundamental constants

Quantity	Symbol	Value[a]	Units
Vacuum permittivity	ε_0	8.85419×10^{-12}	F m^{-1}
Speed of light	c	2.99792×10^{8}	m s^{-1}
Electron charge	q	1.60219×10^{-19}	C
Electron rest mass	m_0	9.10953×10^{-31}	kg
Proton rest mass	M_0	1.67265×10^{-27}	kg
Boltzmann constant	k_B	1.38066×10^{-23}	J K^{-1}
Planck constant	h	6.62616×10^{-34}	J s
Reduced Planck c.	$\hbar$	1.05459×10^{-34}	J s
Atomic radius	r_a	$\sim 10^{-10}$	m
Electron radius	r_e	2.81794×10^{-15}	m

[a]The ratio between the proton and electron rest masses is $M_0/m_0 \simeq 1836$. The vacuum permeability is found from $\mu_0 = 1/(c^2\varepsilon_0)$

Table D.2 Greek alphabet

Small	Capital[a]	Name	Small	Capital	Name
α	A	Alpha	ν	N	Nu, ni
β	B	Beta	ξ	$\varXi$	Xi
γ	$\varGamma$	Gamma	o	O	Omicron
δ	$\varDelta$	Delta	π	$\varPi$	Pi
ε	E	Epsilon	ϱ	P	Rho
ζ	Z	Zeta	σ	$\varSigma$	Sigma
η	H	Eta	τ	T	Tau
θ, ϑ	$\varTheta$	Theta	υ	$\varUpsilon$	Upsilon
ι	I	Iota	ϕ, φ	$\varPhi$	Phi
κ	K	Kappa	χ	X	Chi
λ	$\varLambda$	Lambda	ψ	$\varPsi$	Psi
μ	M	Mu, mi	ω	$\varOmega$	Omega

[a]Symbol ∇ is not a Greek letter. However, its name *nabla* is a Greek word, meaning "harp"

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Solutions

Problems of Chap. 1

1.1 The distance between A and B is a functional of y:

$$G[y] = \int_{AB} \sqrt{\mathrm{d}x^2 + \mathrm{d}y^2} = \int_a^b \sqrt{1 + \dot{y}^2}\,\mathrm{d}x.$$

As $g(y, \dot{y}, x) = \sqrt{1 + \dot{y}^2}$ it is $\partial g / \partial y = 0$, whence the Euler–Lagrange equation reads

$$0 = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial g}{\partial \dot{y}} = \frac{\mathrm{d}}{\mathrm{d}x}\frac{2\dot{y}}{2\,g} = \frac{\ddot{y}g - \dot{y}(2\dot{y}\ddot{y}/2\,g)}{g^2} = \frac{\ddot{y}}{g^3}\,(g^2 - \dot{y}^2) = \frac{\ddot{y}}{g^3},$$

that is, $\ddot{y} = 0$, $y = c_1 x + c_2$. The two constants are found from $c_1 a + c_2 = y_a$, $c_1 b + c_2 = y_b$.

1.2 Letting $H = E$ one finds

$$\frac{x^2}{a^2} + \frac{p^2}{b^2} = 1, \qquad a = \sqrt{2E/c}, \quad b = \sqrt{2\,mE}.$$

The curves are ellipses whose axes are proportional to $\sqrt{E}$. The area of each ellipse is $\pi\,a\,b = 2\,\pi\,E/\omega$, with $\omega = \sqrt{c/m}$. As shown in Sect. 3.3, ω is the angular frequency of the oscillator, so that the area becomes $E\,T$, with $T = 2\,\pi/\omega$ the period. As time evolves, the phase point follows the curve in the clockwise direction; in fact, as the phase point reaches the maximum elongation $x_M > 0$ from the left, the momentum at x_M changes from positive to negative.

1.3 Letting $H = E$ one finds for the maximum elongation $x_M = (s\,E/c)^{1/s}$. Note that the units of c depend on the value of s. The form of the constant-energy curves becomes more and more rectangular as s increases. As in the previous exercise, the phase point follows the curve in the clockwise direction.

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Problems of Chap. 2

2.1 From (2.49) one finds

$$J(E) = \sqrt{m\,c}\oint \sqrt{2E/c - x^2}\,\mathrm{d}x,$$

where the integration path is the ellipse described in Problem 1.2. Letting $x = \sqrt{2\,E/c}\,\sin\varphi$ transforms the above into

$$J(E) = 2\sqrt{\frac{m}{c}}\,E\int_0^{2\pi}\cos^2\varphi\,\mathrm{d}\varphi = \frac{2\pi}{\omega}\,E, \qquad \omega = \sqrt{\frac{c}{m}}.$$

The first of (2.51) then yields $\nu = \dot{w} = \partial H/\partial J = \partial E/\partial J = \omega/(2\pi)$.

Problems of Chap. 3

3.1 Like in problem 1.3, letting $H = E > 0$ one finds for the maximum elongation $x_M = (s\,E/c)^{1/s}$, where the units of c depend on the value of s. The motion is limited to the interval $[-x_M, +x_M]$ and the potential energy is symmetric with respect to the origin. Using (2.47) and exploiting the symmetry yields

$$T = 4\sqrt{\frac{m}{2}}\int_0^{x_M}\frac{\mathrm{d}x}{\sqrt{E - V(x)}} = \sqrt{\frac{8\,m}{E}}\int_0^{x_M}\left[1 - (x/x_M)^s\right]^{-1/2}\,\mathrm{d}x.$$

Letting $\xi = x/x_M$ and using (C.99, C.100) yields

$$T = \sqrt{\frac{8\,m}{E}}\,x_M\int_0^1\frac{\mathrm{d}\xi}{\sqrt{1-\xi^s}} = \sqrt{8\,\pi\,m}\,\frac{(1/s)\,\Gamma(1/s)}{\Gamma(1/s + 1/2)}\left(\frac{s}{c}\right)^{1/s}E^{1/s-1/2}.$$

The result shows that the case $s = 2$, namely, that of the linear harmonic oscillator, is special. In fact, the period does not depend on the total energy, whereas for $s \neq 2$ it does. Still in the case $s = 2$ one finds $T = 2\pi/\omega$, $\omega = \sqrt{c/m}$, as should be (compare with the results of Sect. 3.3). In turn, the case $s \to \infty$ yields $s^{1/s} \to 1$, $c^{1/s} \to 1$ whence, using (C.101), $\lim_{s\to\infty} T = \sqrt{8\,m/E}$. The above is the period in a square well of length 2 (compare with the description of Sect. 3.2). In fact, as $s \to \infty$, the potential energy $c|x|^s/s$ transforms into a square well with $x_M = 1$. The potential energy is shown in Fig. D.1 for some values of s. Thanks to the result of this problem one may tune the form of the potential energy to make the period proportional to a chosen power $h = 1/s - 1/2 \geq -1/2$ of the energy. For instance, letting $s = 2/3$ makes T proportional to E, namely, $T = \sqrt{m/(3c^3)}\,2\pi\,E$.

3.2 The solution is similar to that of Problem 3.1. Letting $H = E < 0$ one finds for the maximum elongation $x_M = [k/(s\,|E|)]^{1/s}$, where the units of k depend on the value of s. The motion is limited to the interval $[-x_M, +x_M]$ and the potential energy is symmetric with respect to the origin. Using (2.47) and exploiting the symmetry yields

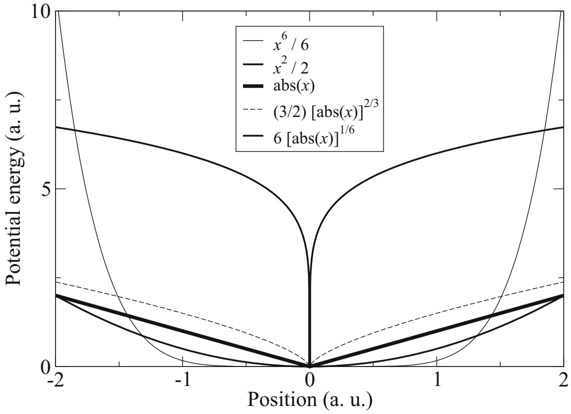


Fig. D.1 Form of the potential energy $c|x|^s/s$ for $c = 1$ and different values of s (Problem 3.1)

$$T = 4\sqrt{\frac{m}{2}} \int_0^{x_M} \frac{\mathrm{d}x}{\sqrt{E - V(x)}} = \sqrt{\frac{8\,m}{|E|}} \int_0^{x_M} \left[(x_M/x)^s - 1\right]^{-1/2} \mathrm{d}x.$$

Letting $\xi = x/x_M$ and using (C.102, C.103) yields

$$T = \sqrt{\frac{8\,m}{|E|}}\, x_M \int_0^1 \frac{\mathrm{d}\xi}{\sqrt{1/\xi^s - 1}} = \sqrt{8\,\pi\,m}\, \frac{\Gamma(1/s + 1/2)}{s\,\Gamma(1/s + 1)} \left(\frac{k}{s}\right)^{1/s} |E|^{-1/s-1/2}.$$

The Coulomb case $s = 1$ yields $T = \sqrt{2\,m}\,\pi\,k\,|E|^{-3/2}$ (in fact, in the Coulomb case and for a closed trajectory the period is always proportional to $|E|^{-3/2}$, compare with (3.81)). Note that in the case considered here the particle crosses the origin because the initial conditions are such that its trajectory is aligned with the x axis. The limit $s \to \infty$ yields $s^{1/s} \to 1$, $c^{1/s} \to 1$ whence, using (C.101, C.103), $\lim_{s\to\infty} T = 0$. The potential energy is shown in Fig. D.2 for some values of s.

3.3 The O reference is chosen as in Sect. 3.13.5, whence $T_{1a} = E = (m_1/m)\,E_B$. From (3.36) one extracts $\mu/s_0 = \tan[(\pi - \chi)/4]$, to find

$$\frac{2\,\mu/s_0}{1 - (\mu/s_0)^2} = \frac{2\,\mu\,s_0}{s_0^2 - \mu^2} = \tan\left(\frac{\pi - \chi}{2}\right) = \frac{1}{\tan(\chi/2)},$$

where s_0 is given by the second of (3.33). It follows that $s_0^2 - \mu^2 = 2\,\lambda\,s_0$ and $\tan(\chi/2) = \lambda/\mu$. Then, noting that (3.23) contains $\sin^2(\chi/2) = \tan^2(\chi/2)/[1 + \tan^2(\chi/2)]$, and using (3.73), one finds $\sin^2(\chi/2) = 1/(1 + c^2/\lambda^2)$. The expression of λ is taken from the first of (3.32), with α given by (3.75). Inserting the result into (3.23) yields

$$T_{1b} = \frac{\alpha^2\,(1 - m_1/m_2)^2 + c^2\,T_{1a}^2}{\alpha^2\,(1 + m_1/m_2)^2 + c^2\,T_{1a}^2}\, T_{1a}, \quad T_{1a} - T_{1b} = \frac{4\,(m_1/m_2)\,T_{1a}}{(1 + m_1/m_2)^2 + (c/\alpha)^2\,T_{1a}^2}.$$

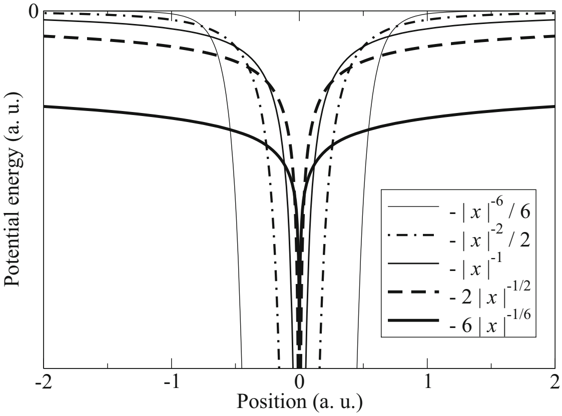


Fig. D.2 Form of the potential energy $-k|x|^{-s}/s$ for $k = 1$ and different values of s (Problem 3.2)

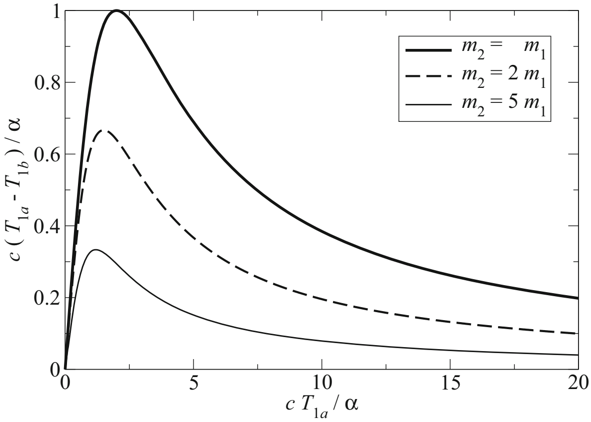


Fig. D.3 Normalized loss of energy $c\,(T_{1a} - T_{1b})/\alpha$ as a function of the normalized initial energy $c\,T_{1a}/\alpha$ (Problem 3.3), for different values of the ratio m_1/m_2

Obviously it is $T_{1b} < T_{1a}$. It follows that $T_{1a} - T_{1b}$ is the loss of energy due to the collision. It is also interesting to note that using the normalized energies $c\,T_{1a}/\alpha$ and $c\,T_{1b}/\alpha$ makes the expressions above to depend on the m_1/m_2 ratio only. The loss of energy is drawn in normalized form in Fig. D.3 for different values of m_1/m_2.

Problems of Chap. 4

4.1 Using primes to indicate derivatives, a first integration yields

$$\varphi' = \varphi'(c) - H, \qquad H(x) = \int_c^x \frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi,$$

where H is integrated by parts:

$$\int_a^x H(\xi)\,\mathrm{d}\xi = x\,H(x) - a\,H(a) - \int_a^x \xi\,\frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi.$$

Integrating φ' and using the expression of $\int_a^x H(\xi)\,\mathrm{d}\xi$ yields the solution

$$\varphi = \varphi(a) + \varphi'(c)\,(x-a) - x\int_c^x \frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi + a\int_c^a \frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi + \int_a^x \xi\,\frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi.$$

4.2 Letting $c = a$ in the solution to Problem 4.1 yields at any point x within $[a, b]$ the expression

$$\varphi(x) = \varphi(a) + \varphi'(a)\,(x-a) - x\int_a^x \frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi + \int_a^x \xi\,\frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi.$$

For $x > b$ it is $\varrho = 0$ so that the solution of $\varphi'' = 0$ is linear and has the form $\varphi(x) = \varphi(b) + \varphi'(b)\,(x-b)$. The term $\varphi(b)$ in the latter is obtained by letting $x = b$ in the above expression of $\varphi(x)$. One finds $\varphi(b) = \varphi(a) + \varphi'(a)\,(b-a) - b\,M_0 + M_1$, with

$$M_0 = \int_a^b \frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi, \qquad M_1 = \int_a^b \xi\,\frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi$$

the first two moments of ϱ/ε_0 (compare with Sect. C.6). The derivative φ' is found from Problem 4.1 with $c = a$, and reads

$$\varphi'(x) = \varphi'(a) - \int_a^x \frac{\varrho(\xi)}{\varepsilon_0}\,\mathrm{d}\xi,$$

whence $\varphi'(b) = \varphi'(a) - M_0$. Using the expressions of $\varphi(b)$, $\varphi'(b)$ thus found yields

$$\varphi(x) = \varphi(a) + \varphi'(a)\,(x-a) - M_0\,x + M_1, \qquad x > b.$$

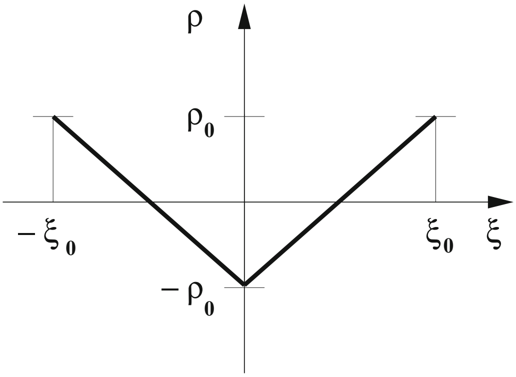
4.3 From the findings of Problem 4.2 one observes that the solution φ is invariant for any charge density $\tilde{\varrho}$ that leaves M_0 and M_1 unchanged. Due to this, if both M_0, M_1 differ from zero, the new charge density must contain two adjustable parameters in order to fit the values of M_0, M_1 through the expressions introduced in Problem 4.2. If only one moment differs from zero, one parameter suffices, while no parameter is necessary if both moments are equal to zero. Figure D.4 gives an example of charge density such that $M_0 = 0$ and $M_1 = 0$.

4.4 The starting point is the solution for $x > b$ found in Problem 4.2. When the charge density is removed, the new solution reads

$$\varphi(x) = \tilde{\varphi}(a) + \tilde{\varphi}'(a)\,(x-a).$$

For $x > b$ the two solutions become equal to each other by letting $\tilde{\varphi}(a) = \varphi(a) - M_0\,a + M_1$ and $\tilde{\varphi}'(a) = \varphi'(a) - M_0$.

Fig. D.4 Example of charge density such that $M_0 = 0$ and $M_1 = 0$



4.5 Considering that the value of h is unknown, the integrals that define the moments (Problem 4.2) must be extended from $-\infty$ to $+\infty$. One finds $\mu = M_0$, $h = M_1/M_0$. If $h \geq a$, the solution is given by $\varphi = \varphi(a) + \varphi'(a)(x - a) - M_0 x + M_1$ for $x \geq h$, while it is given by $\varphi = \varphi(a) + \varphi'(a)(x - a)$ for $x < h$. If $h < a$, the solution is given by $\varphi = \varphi(a) + \varphi'(a)(x - a)$ for $x \geq h$, while it is given by $\varphi = \varphi(a) + \varphi'(a)(x - a) - M_0 x + M_1$ for $x < h$. At h the electric potential is continuous, $\varphi(h^+) = \varphi(h^-) = \varphi(a) + \varphi'(a)(h - a)$, whereas the electric field is discontinuous, $\varphi'(h^-) - \varphi'(h^+) = M_0$. The case $M_0 \neq 0$, $M_1 = 0$ yields $\mu = M_0$, $h = 0$, while the case $M_0 = 0$, $M_1 \neq 0$ can not be fulfilled by $\mu\,\delta(x - h)$.

Problems of Chap. 5

5.1 From $n = n(x_1)$ one finds that grad$n = \mathbf{i}_1\,\mathrm{d}n/\mathrm{d}x_1$ is parallel to x_1 whereas $\mathrm{d}n/\mathrm{d}x_2 = \mathrm{d}n/\mathrm{d}x_3 = 0$. From the eikonal Eq. (5.57) it follows

$$\frac{\mathrm{d}}{\mathrm{d}s}\left(n\,\frac{\mathrm{d}x_2}{\mathrm{d}s}\right) = 0, \qquad \frac{\mathrm{d}}{\mathrm{d}s}\left(n\,\frac{\mathrm{d}x_3}{\mathrm{d}s}\right) = 0,$$

whence $n\,\mathrm{d}x_2/\mathrm{d}s = \text{const}$, $n\,\mathrm{d}x_3/\mathrm{d}s = \text{const}$. The ratio of the latter relations yields $\mathrm{d}x_2/\mathrm{d}x_3 = \text{const}$, namely, $x_2 = a x_3 + b$, where a, b are constants. This expression is one of the two parametric equations $u(x_1, x_2, x_3) = 0$, $v(x_1, x_2, x_3) = 0$ describing the ray, and shows that the ray belongs to a plane parallel to x_1. By a suitable rotation around x_1, such that $x_2 \to x_2'$, $x_3 \to x_3'$, the plane of the ray is made parallel to the plane $x_1\,x_2'$, so that the third coordinate x_3' is fixed. In the new reference, let ϑ be the angle between the direction of the ray and x_1 at some point P; it is $\mathrm{d}x_1 = \cos\vartheta\,\mathrm{d}s, \mathrm{d}x_2' = \sin\vartheta\,\mathrm{d}s$. The eikonal equation in the new reference then provides

$$n\,\frac{\mathrm{d}x_2'}{\mathrm{d}s} = \text{const}, \qquad n\,\sin\vartheta = \text{const}.$$

5.2 Like in Problem 5.1 one considers the case where the refraction index depends only on the x_1 coordinate. Let the medium be made of three regions separated by two planes parallel to each other.

The two external regions A and B have a constant refraction index, n_A and, respectively, $n_B \neq n_A$. The internal region I, whose thickness is s, has a refraction index that varies continuously from n_A to n_B as x_1 varies from the A-I interface to the I-B interface. Applying the solution of Problem 5.1 to this case shows that $n_A \sin\vartheta_A = \text{const}$ everywhere in region A, hence the ray is a straight line there; similarly it is $n_B \sin\vartheta_B = \text{const}$ everywhere in region B, with the same constant. It follows

$$n_B \sin\vartheta_B = n_A \sin\vartheta_A .$$

Unless $\vartheta_A = 0$, the position of the ray along the x_2' axis at the I-B interface is different from that at the A-I interface; if, however, s is made to vanish, the position becomes the same, this yielding the *Descartes law of refraction*: the ray crossing an interface between two media is continuous, whereas its slopes on the two sides of the interface fulfill (D). The result still holds in the cases where the interface between the two media is not planar, provided its curvature is small enough to make geometrical optics applicable.

Problems of Chap. 6

6.1 Letting $\vartheta = \beta\, h\, \nu$, with $\beta = 1/(k_B T)$, the Boltzmann distribution takes the form $N_n = N_0 \exp(-n\,\vartheta)$, whence

$$\sum_{n=0}^{\infty} N_n = N_0 \left[1 + \exp(-\vartheta) + \exp(-2\,\vartheta) + \ldots\right] = \frac{N_0}{1 - \exp(-\vartheta)},$$

and

$$\sum_{n=0}^{\infty} n\, h\, \nu\, N_n = h\, \nu\, N_0 \left[\exp(-\vartheta) + 2\, \exp(-2\,\vartheta) + 3\, \exp(-3\,\vartheta) + \ldots\right].$$

Observing that $n \exp(-n\,\vartheta) = -\mathrm{d} \exp(-n\,\vartheta)/\mathrm{d}\vartheta$, one finds

$$\sum_{n=0}^{\infty} n\, h\, \nu\, N_n = -h\, \nu\, \frac{\mathrm{d}}{\mathrm{d}\vartheta} \left(\sum_{n=0}^{\infty} N_n - N_0\right) = h\, \nu\, \frac{N_0 \exp(-\vartheta)}{\left[1 - \exp(-\vartheta)\right]^2},$$

whence

$$\overline{E}_n = \frac{\sum_{n=0}^{\infty} n\, h\, \nu\, N_n}{\sum_{n=0}^{\infty} N_n} = \frac{h\, \nu}{\exp(\vartheta) - 1} = \frac{h\, \nu}{\exp(\beta\, h\, \nu) - 1}.$$

Problems of Chap. 8

8.1 Consider the homogeneous equation associated to (8.76), $g'' + a\,g' + b\,g = 0$, and let $f = g\,h$ and $u = h'$; this splits (8.76) into the system

$$g'' + a\,g' + b\,g = 0, \qquad g\,u' + (2\,g' + a\,g)\,u = c.$$

If g is known, then u is found by integrating a first-order equation, whence $f = g\int u\,\mathrm{d}\xi$. To find g one lets $A(x) = \int a\,\mathrm{d}\xi$, $g = \exp(-A/2)\,w$, this transforming the homogeneous equation for g into

$$w'' + q\,w = 0, \qquad q = b - a^2/4 - a'/2,$$

which is a time-independent Schrödinger equation.

Problems of Chap. 9

9.1 Inserting the expression of c_k into the one-dimensional form of (9.26) yields

$$A\,(x - u\,t\,;k_0) = \frac{\sqrt{\sigma/2}}{\pi^{3/4}} \int_{-\infty}^{+\infty} \exp\left[\mathrm{i}\ (x - u\,t)\ (k - k_0) - \sigma^2\,k^2/2\right] \mathrm{d}k.$$

Following the same procedure as in Sect. C.8 one finds

$$\mathrm{i}\ (x - u\,t)\ (k - k_0) - \frac{1}{2}\,\sigma^2\,k^2 = -\frac{(x - u\,t)^2}{2\,\sigma^2} - \frac{\sigma^2}{2}\left(k - j\,\frac{x - u\,t}{\sigma^2}\right)^2,$$

whence

$$A\,(x - u\,t\,;k_0) = \frac{1}{\pi^{1/4}\sqrt{\sigma}} \exp\left[-\mathrm{i}\,k_0\ (x - u\,t) - \frac{(x - u\,t)^2}{2\,\sigma^2}\right].$$

The particle's localization is determined by

$$|A(x - u\,t)|^2 = \frac{1}{\sqrt{\pi}\,\sigma} \exp\left[-\frac{(x - u\,t)^2}{\sigma^2}\right].$$

Using again the results of Sect. C.8 yields $||A|| = 1$.

9.2 Remembering that $|\psi|^2 = |A|^2$, the one-dimensional form of (9.23) reads

$$x_0(t) = \int_{-\infty}^{+\infty} x\,|A|^2\,\mathrm{d}x = \int_{-\infty}^{+\infty} (x - u\,t)\,|A|^2\,\mathrm{d}x + u\,t \int_{-\infty}^{+\infty} |A|^2\,\mathrm{d}x.$$

Letting $s = x - u\,t$ one finds that the integral of $s\,|A(s)|^2$ vanishes because the integrand is odd and the integration domain is symmetric with respect to the origin. Using the result $||A|| = 1$ of Problem 9.1 then yields $x_0(t) = u\,t$.

Problems of Chap. 10

10.1 To determine the time evolution of the expectation value of the wavepacket for a free particle one starts from the general expression (9.5), with $w_{\mathbf{k}}(\mathbf{r})$ and $E_{\mathbf{k}} = \hbar\,\omega_{\mathbf{k}}$ given by (9.22), and $c_{\mathbf{k}}$ given by the second relation in (9.6). The wave function is assumed normalized, $\int_{-\infty}^{+\infty} |\psi(\mathbf{r},t)|^2\,\mathrm{d}^3r = \int_{-\infty}^{+\infty} |c(\mathbf{k})|^2\,\mathrm{d}^3k = 1$. Using the first spatial coordinate x_1 and defining $m_{\mathbf{k}} = c_{\mathbf{k}}\,\exp(-\mathrm{i}\,\omega_{\mathbf{k}}\,t)$, the following are of use: $x_1\,w_{\mathbf{k}} = -\mathrm{i}\,\partial w_{\mathbf{k}}/\partial k_1$, $x_1^2\,w_{\mathbf{k}} = -\partial^2 w_{\mathbf{k}}/\partial k_1^2$, and

$$-\int_{-\infty}^{+\infty} m_{\mathbf{k}}\,\frac{\partial w_{\mathbf{k}}}{\partial k_1}\,\mathrm{d}k_1 = \int_{-\infty}^{+\infty} w_{\mathbf{k}}\,\frac{\partial m_{\mathbf{k}}}{\partial k_1}\,\mathrm{d}k_1, \int_{-\infty}^{+\infty} m_{\mathbf{k}}\,\frac{\partial^2 w_{\mathbf{k}}}{\partial k_1^2}\,\mathrm{d}k_1 = \int_{-\infty}^{+\infty} w_{\mathbf{k}}\,\frac{\partial^2 m_{\mathbf{k}}}{\partial k_1^2}\,\mathrm{d}k_1,$$

where the last two equalities are obtained by integrating by parts and observing that, due to the normalization condition, $c_{\mathbf{k}}$ and $\partial c_{\mathbf{k}}/\partial k_1$ vanish at infinity. In turn,

$$\mathrm{i}\,\frac{\partial m_{\mathbf{k}}}{\partial k_1} = \left(u_1\,t\,c_{\mathbf{k}} + \mathrm{i}\,\frac{\partial c_{\mathbf{k}}}{\partial k_1}\right)\exp(-\mathrm{i}\,\omega_{\mathbf{k}}\,t), \qquad u_1 = \frac{\partial \omega_{\mathbf{k}}}{\partial k_1} = \frac{\hbar\,k_1}{m},$$

$$-\frac{\partial^2 m_{\mathbf{k}}}{\partial k_1^2} = \left[\left(u_1^2\,t^2 + \mathrm{i}\,\frac{\hbar}{m}\,t\right)c_{\mathbf{k}} + 2\,\mathrm{i}\,u_1\,t\,\frac{\partial c_{\mathbf{k}}}{\partial k_1} - \frac{\partial^2 c_{\mathbf{k}}}{\partial k_1^2}\right]\exp(-\mathrm{i}\,\omega_{\mathbf{k}}\,t).$$

The expectation value $\langle x_1\rangle = \langle\psi|x_1|\psi\rangle$ involves an integration over $\mathbf{r}$ to calculate the scalar product, an integration over $\mathbf{k}$ to calculate the integral expression of ψ, and an integration over $\mathbf{k}'$ to calculate the integral expression of ψ^*. Performing the integration over $\mathbf{r}$ first, letting $c'_{\mathbf{k}} = c(\mathbf{k}')$, $\omega'_{\mathbf{k}} = \omega(\mathbf{k}')$, and using (C.56) yields

$$\langle x_1\rangle = \iiint_{-\infty}^{+\infty}\left(u_1\,t\,|c_{\mathbf{k}}|^2 + \mathrm{i}\,c_{\mathbf{k}}^*\,\frac{\partial c_{\mathbf{k}}}{\partial k_1}\right)\mathrm{d}^3k.$$

Letting $c_{\mathbf{k}} = a_{\mathbf{k}} + \mathrm{i}\,b_{\mathbf{k}}$, with $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ real, and using the asymptotic vanishing of $c_{\mathbf{k}}$, one finds

$$\iiint_{-\infty}^{+\infty}\mathrm{i}\,c_{\mathbf{k}}^*\,\frac{\partial c_{\mathbf{k}}}{\partial k_1}\,\mathrm{d}^3k = x_{01}, \qquad x_{01} = \iiint_{-\infty}^{+\infty}\left(\frac{\partial a_{\mathbf{k}}}{\partial k_1}\,b_{\mathbf{k}} - \frac{\partial b_{\mathbf{k}}}{\partial k_1}\,a_{\mathbf{k}}\right)\mathrm{d}^3k,$$

where x_{01} is a real constant. Repeating the calculation for x_2 and x_3, and letting $\mathbf{u} = \mathrm{grad}_{\mathbf{k}}\omega$, $\mathbf{r}_0 = (x_{01}, x_{02}, x_{03})$, finally yields

$$\langle\mathbf{r}\rangle = \mathbf{r}_0 + \iiint_{-\infty}^{+\infty}\mathbf{u}\,t\,|c_{\mathbf{k}}|^2\,\mathrm{d}^3k, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle\mathbf{r}\rangle = \iiint_{-\infty}^{+\infty}\mathbf{u}\,|c_{\mathbf{k}}|^2\,\mathrm{d}^3k = \text{const.}$$

If $|c_{\mathbf{k}}|^2$ is even with respect to all components of $\mathbf{k}$, the expectation value of $\mathbf{r}$ does not change with respect to the initial value $\mathbf{r}_0$. Otherwise, it moves at constant speed.

10.2 The time evolution of the standard deviation of position is found following the same line and using the same symbols and relations as in Problem 10.1, starting with

$$\langle x_1^2\rangle = \iiint_{-\infty}^{+\infty} \left[\left(u_1^2\,t^2 + \mathrm{i}\,\frac{\hbar}{m}\,t\right)\,|c_{\mathbf{k}}|^2 + 2\mathrm{i}\,u_1\,t\,c_{\mathbf{k}}^*\,\frac{\partial c_{\mathbf{k}}}{\partial k_1} - c_{\mathbf{k}}^*\,\frac{\partial^2 c_{\mathbf{k}}}{\partial k_1^2}\right]\mathrm{d}^3k.$$

An integration by parts combined with the normalization condition for $c_{\mathbf{k}}$ shows that

$$\iiint_{-\infty}^{+\infty} 2\mathrm{i}\,u_1\,t\,c_{\mathbf{k}}^*\,\frac{\partial c_{\mathbf{k}}}{\partial k_1}\,\mathrm{d}^3k = -\mathrm{i}\,\frac{\hbar}{m}\,t + 2\,t\iiint_{-\infty}^{+\infty} u_1\,\left(\frac{\partial a_{\mathbf{k}}}{\partial k_1}\,b_{\mathbf{k}} - \frac{\partial b_{\mathbf{k}}}{\partial k_1}\,a_{\mathbf{k}}\right)\mathrm{d}^3k,$$

where the second term at the right hand side is real, whereas the first one cancels out in the expression of $\langle x_1^2\rangle$. Finally, another integration by parts yields

$$-\iiint_{-\infty}^{+\infty} c_{\mathbf{k}}^*\,\frac{\partial^2 c_{\mathbf{k}}}{\partial k_1^2}\,\mathrm{d}^3k = \iiint_{-\infty}^{+\infty}\left|\frac{\partial c_{\mathbf{k}}}{\partial k_1}\right|^2\mathrm{d}^3k.$$

In conclusion,

$$\langle x_1^2\rangle = \iiint_{-\infty}^{+\infty}\left|u_1\,t\,c_{\mathbf{k}} + \mathrm{i}\,\frac{\partial c_{\mathbf{k}}}{\partial k_1}\right|^2\mathrm{d}^3k.$$

Repeating the calculation for x_2 and x_3 yields

$$\langle \mathbf{r}\cdot\mathbf{r}\rangle = \int_{-\infty}^{+\infty}\left|\mathbf{u}\,t\,c_{\mathbf{k}} + \mathrm{i}\,\mathrm{grad}_{\mathbf{k}}c_{\mathbf{k}}\right|^2\mathrm{d}^3k,$$

where the definition of the squared length of a complex vector is found in (A.2) and (A.4). The standard deviation of the wave packet in the $\mathbf{r}$ space is the positive square root of $\langle\mathbf{r}\cdot\mathbf{r}\rangle - \langle\mathbf{r}\rangle\cdot\langle\mathbf{r}\rangle = \sum_{i=1}^{3}(\Delta x_i)^2$, where the expression of $\langle\mathbf{r}\rangle$ was derived in Prob. 10.1. It is easily shown that the standard deviation diverges with t. In fact, the leading term of $\langle x_1^2\rangle$ and, respectively, $\langle x_1\rangle^2$ is

$$\langle x_1^2\rangle \sim t^2\iiint_{-\infty}^{+\infty} u_1^2\,|c_{\mathbf{k}}|^2\,\mathrm{d}^3k, \qquad \langle x_1\rangle^2 \sim t^2\left(\iiint_{-\infty}^{+\infty} u_1\,|c_{\mathbf{k}}|^2\,\mathrm{d}^3k\right)^2,$$

the first of which is positive, whereas the second one is non negative. Letting $f = c_{\mathbf{k}}$, $g = u_1 c_{\mathbf{k}}$ in the Schwartz inequality (8.15) and using the normalization condition of $c_{\mathbf{k}}$ yields

$$\iiint_{-\infty}^{+\infty} u_1^2|c_{\mathbf{k}}|^2\,\mathrm{d}^3k > \left(\iiint_{-\infty}^{+\infty} u_1|c_{\mathbf{k}}|^2\,\mathrm{d}^3k\right)^2,$$

where the strict inequality holds because f and g are not proportional to each other. For the leading term it follows that $(\Delta x_1)^2 = \langle x_1^2\rangle - \langle x_1\rangle^2 \sim \mathrm{const}\times t^2$, where the constant is strictly positive. The same reasoning applies to x_2, x_3. In conclusion, the standard deviation Δx_i associated with the ith coordinate diverges in time with the first power of t.

10.3 Still with reference to the wave packet of a free particle used in Problems 10.1 and 10.2, the time evolution of the expectation value in the $\mathbf{p}$ space is found starting with the first component p_1 of momentum. The corresponding operator is $\hat{p}_1 = -\mathrm{i}\hbar\,\partial/\partial x_1$, and the following relations are of use: $\hat{p}_1 w_{\mathbf{k}} = \hbar\,k_1\,w_{\mathbf{k}}$, $\hat{p}_1^2 w_{\mathbf{k}} = \hbar^2\,k_1^2\,w_{\mathbf{k}}$. The expectation value $\langle p_1\rangle = \langle\psi|p_1|\psi\rangle$ involves an integration over $\mathbf{r}$ to calculate the scalar product, an integration over $\mathbf{k}$ to calculate the integral expression of ψ, and an integration over $\mathbf{k}'$ to calculate the integral expression of ψ^*. Performing the integration over $\mathbf{r}$ first, letting $c'_{\mathbf{k}} = c(\mathbf{k}')$, $\omega'_{\mathbf{k}} = \omega(\mathbf{k}')$, and using (C.56) yields

$$\langle p_1\rangle = \iiint_{-\infty}^{+\infty} \hbar\,k_1\,|c_{\mathbf{k}}|^2\,\mathrm{d}^3k = p_{01}.$$

The real constant p_{01} defined above is independent of time. In conclusion, repeating the calculation for p_2 and p_3, and letting $\mathbf{p}_0 = (p_{01}, p_{02}, p_{03})$, the following holds: $\langle\mathbf{p}\rangle = \mathbf{p}_0$. If $|c_{\mathbf{k}}|^2$ is even with respect to all components of $\mathbf{k}$, the expectation value of $\mathbf{p}$ is zero.

10.4 The calculation of $\langle\psi|\hat{p}_1^2|\psi\rangle$ is carried out following the same line as in Problem 10.3, leading to

$$\langle p_1^2\rangle = \iiint_{-\infty}^{+\infty} \hbar^2\,k_1^2\,|c_{\mathbf{k}}|^2\,\mathrm{d}^3k.$$

Repeating the calculation for x_2 and x_3 yields

$$\langle\mathbf{p}\cdot\mathbf{p}\rangle = \iiint_{-\infty}^{+\infty} \hbar\,\mathbf{k}\cdot\hbar\,\mathbf{k}\;|c_{\mathbf{k}}|^2\;\mathrm{d}^3k.$$

In turn, the standard deviation of the wave packet in the $\mathbf{p}$ space is the positive square root of $\langle\mathbf{p}\cdot\mathbf{p}\rangle - \langle\mathbf{p}\rangle\cdot\langle\mathbf{p}\rangle = \sum_{i=1}^{3}(\Delta p_i)^2$. Letting $f = c_{\mathbf{k}}$, $g = \hbar k_1 c_{\mathbf{k}}$ in the Schwartz inequality (8.15) and using the normalization condition of $c_{\mathbf{k}}$ yields

$$\iiint_{-\infty}^{+\infty} \hbar^2\,k_1^2\,|c_{\mathbf{k}}|^2\,\mathrm{d}^3k > \left(\iiint_{-\infty}^{+\infty} \hbar\,k_1\,|c_{\mathbf{k}}|^2\,\mathrm{d}^3k\right)^2,$$

where the strict inequality holds because f and g are not proportional to each other. It follows that $(\Delta p_1)^2 = \langle p_1^2\rangle - \langle p_1\rangle^2$ is strictly positive and constant in time. The same reasoning applies to p_2, p_3. In conclusion, the standard deviation Δp_i associated with the ith component of momentum is constant in time.

10.5 One finds $\langle x\rangle = x_0$, $\mathrm{d}\hbar\,\beta/\mathrm{d}x = \hbar\,k_0$, $\langle p_e\rangle = \hbar\,k_0$,

$$\left\langle\frac{p_e^2}{2\,m}\right\rangle = \frac{\hbar^2\,k_0^2}{2\,m}, \qquad \langle Q\rangle = \frac{\hbar^2}{8\,m\,\sigma^2}, \qquad \langle T\rangle = \frac{\hbar^2}{2\,m}\left(k_0^2 + \frac{1}{4\,\sigma^2}\right).$$

One notes that for a fixed $\langle T\rangle$ all non-negative values of the "convective" and "thermal" parts that add up to $\langle T\rangle$ are allowed. In the particular case of a free particle, where $\langle T\rangle = \langle E\rangle$, the above shows that different values of the average momentum and "dispersion" may combine to yield the same total energy.

Problems of Chap. 11

11.1 Letting $b^- = \pi\, a\, \sqrt{2\, m}\,(\sqrt{E} - \sqrt{E - V_0})/\hbar$, $b^+ = \pi\, a\, \sqrt{2\, m}\,(\sqrt{E} + \sqrt{E - V_0})/\hbar$ and remembering that $\sinh b \simeq b$ when $|b| \ll 1$ yields, with m fixed,

$$R(a \to 0) = \left(\frac{b^-}{b^+}\right)^2 = \frac{(\sqrt{E} - \sqrt{E - V_0})^2}{(\sqrt{E} + \sqrt{E - V_0})^2},$$

that coincides with the first relation in (11.11). Conversely, when $a > 0$ is fixed and m is let grow one finds

$$R \simeq \exp\left[2\,(b^- - b^+)\right] = \exp\left(-4\,\pi\, a\, \sqrt{2\, m}\, \sqrt{E - V_0}/\hbar\right),$$

namely, $\lim_{m\to\infty} R = 0$, this recovering the classical limit.

11.2 The maximum of the cotangent's argument $s\,\sqrt{2\, m\,(E - V_0)/\hbar^2}$ is found by letting $E = 0$. Thus,

$$\gamma = \frac{s}{\hbar}\,\sqrt{-2\, m\, V_0} \simeq 13.4, \qquad \frac{13.4}{\pi} \simeq 4.3.$$

As a consequence, the cotangent has four complete branches and one incomplete branch in the interval $V_0 < E < 0$, corresponding to five eigenvalues $E_1, \dots, E_5$. Using the normalized parameter $0 < \eta = \sqrt{1 - E/V_0} < 1$, the equation to be solved reads

$$\frac{\eta^2 - 1/2}{\eta\,\sqrt{1 - \eta^2}} = \cot\,(\gamma\, \eta)\,.$$

Over the η axis, the 5 branches belong to the intervals $(0, \pi/\gamma)$, $(\pi/\gamma, 2\pi/\gamma)$, $(2\pi/\gamma, 3\pi/\gamma)$, $(3\pi/\gamma, 4\pi/\gamma)$, $(4\pi/\gamma, 1)$.

Problems of Chap. 13

13.1 Letting $Z = 1$ one finds that the lowest total energy of the electron in the hydrogen atom has the value

$$E_1(Z = 1) = -\frac{m_0}{2\,\hbar^2}\left(\frac{q^2}{4\,\pi\,\varepsilon_0}\right)^2.$$

As noted in Sect. 13.5.2, the electron is bound as long as $E < 0$. As a consequence, the minimum energy for which it becomes free is $\lim_{n\to\infty} E_n = 0$. The hydrogen atom's ionization energy is thus found to be

$$E_{\rm ion} = 0 - E_1(Z = 1) = |E_1(Z = 1)| = \frac{m_0}{2\,\hbar^2}\left(\frac{q^2}{4\,\pi\,\varepsilon_0}\right)^2.$$

Replacing the constants' values of Table D.1 yields $E_{\rm ion} \simeq 2.18 \times 10^{-18}$ J $\simeq 13.6$ eV.

13.2 The time-dependent wave function is in this case $\psi = w(E_{\min}) \exp(-\mathrm{i}\, E_{\min}\, t/\hbar)$, whence $|\psi|^2 = \exp(-2\,r/a)/(\pi\, a^3)$. Taking the Jacobian determinant $J = r^2 \sin\vartheta$ from (B.3) and using the definitions of Sect. 10.5 one finds

$$\langle r\rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} r\, \frac{\exp(-2\,r/a)}{\pi\, a^3}\, r^2 \sin\vartheta\, \mathrm{d}r\, \mathrm{d}\vartheta\, \mathrm{d}\varphi = \frac{3}{2}\, a.$$

From (13.89) one finds $a_1 = a(Z=1) = 4\,\pi\,\hbar^2\,\varepsilon_0/(m_0\, q^2) \simeq 5.3\times 10^{-11}$ m $\simeq 0.53$ Å, where the constants' values are taken from Table D.1. Note that $a_1 = r_1/2$, with r_1 is the radius of the ground state derived from the Bohr hypothesis (Sect. 7.4.4). The expectation value of r turns out to be $\langle r\rangle \simeq 0.8$ Å.

Problems of Chap. 14

14.1 From $h^{(0)}_{\mathbf{bg}} = [A/(2\,\pi)^3]/(q_c^2 + q^2)$ and $q = |\mathbf{b} - \mathbf{g}|$ one finds

$$H^{(0)}_{\mathbf{b}}(E_{\mathbf{g}}) = \frac{A^2}{(2\,\pi)^6} \int_0^\pi \int_0^{2\pi} \frac{1}{(q_c^2 + q^2)^2} \sin\vartheta\, \mathrm{d}\vartheta\, \mathrm{d}\varphi,$$

$A = \kappa\, Z\, e^2/\varepsilon_0$. Observing that $\mathbf{b}$ is a fixed vector one can use it as the reference for angle ϑ, so that $q^2 = (\mathbf{b} - \mathbf{g})\cdot(\mathbf{b} - \mathbf{g}) = b^2 + g^2 - 2\,b\,g\,\cos\vartheta$. From $g = b$ it follows $q^2 = 4\,g^2 \sin^2(\vartheta/2)$. On the other hand it is $\sin\vartheta\, \mathrm{d}\vartheta = \mathrm{d}\sin^2(\vartheta/2)$ whence, integrating over φ and letting $\mu = \sin^2(\vartheta/2)$,

$$H^{(0)}_{\mathbf{b}}(E_{\mathbf{g}}) = \frac{A^2}{(2\,\pi)^5} \int_0^1 \frac{\mathrm{d}\mu}{(q_c^2 + 4\,g^2\,\mu)^2} = \frac{A^2/(2\,\pi)^5}{q_c^2\,(q_c^2 + 4\,g^2)}.$$

The dependence on $E_{\mathbf{g}}$ is found through the relation $E_{\mathbf{g}} = \hbar^2\, g^2/(2\,m)$.

Problems of Chap. 15

15.1 After selecting a number $0 < \eta < 1/2$, define E^+ and E^- such that $P(E^+) = \eta$, $P(E^-) = 1 - \eta$. It follows

$$E^+ - E^- = 2\,k_B\,T\, \log\frac{1-\eta}{\eta}.$$

Letting, e.g., $\eta = 0.1$ one finds $E(P = 0.9) - E(P = 0.1) = 2\,k_B\,T\, \log 9 \simeq 4.39\,k_B\,T$. Similarly, letting $\eta = 0.01$ one finds $E(P = 0.99) - E(P = 0.01) = 2\,k_B\,T\, \log 99 \simeq 9.19\,k_B\,T$. At $T = 300$ K it is $k_B\,T \simeq 25.8$ meV. From the above results one finds $E(P = 0.9) - E(P = 0.1) \simeq 113$ meV and $E(P = 0.99) - E(P = 0.01) \simeq 237$ meV, respectively.

Problems of Chap. 19

19.1 Using (19.115) and adding up the two expressions in (19.118) one finds

$$\mu_p = q \left(\frac{m_{hh}^{1/2}}{m_{hh}^{3/2} + m_{hl}^{3/2}} + \frac{m_{hl}^{1/2}}{m_{hh}^{3/2} + m_{hl}^{3/2}} \right) \tau_p = \frac{q\,\tau_p}{\overline{m}_h}.$$

Using the values taken from Table 17.3 yields

$$\frac{m_0}{\overline{m}_h} = \frac{0.5^{1/2}}{0.5^{3/2} + 0.16^{3/2}} + \frac{0.16^{1/2}}{0.5^{3/2} + 0.16^{3/2}},$$

whence $\overline{m}_h \simeq 0.377\, m_0$. As for a_p, using the common value of the relaxation time in (19.122) yields

$$a_p = \frac{q\,\tau_p}{\mu_p^2} \left(\frac{\mu_{ph}}{m_{hh}} + \frac{\mu_{pl}}{m_{hl}} \right).$$

Replacing the expressions (19.118) of μ_{ph}, μ_{pl},

$$a_p = \frac{m_{hh}^{3/2} + m_{hl}^{3/2}}{m_{hh}^{1/2}\, m_{hl}^{1/2} \left(m_{hh}^{1/2} + m_{hl}^{1/2} \right)} = \frac{0.5^{3/2} + 0.16^{3/2}}{0.5^{1/2}\ 0.16^{1/2} \left(0.5^{1/2} + 0.16^{1/2} \right)} \simeq 1.33.$$

Problems of Chap. 21

21.1 Using $k_B\,T/q \simeq 26$ mV (compare with (19.162)) and $n_i \simeq 10^{10}$ cm^{-3} (Table 18.2), one finds

$$\psi_0 = \frac{k_B\,T}{q} \log \left(\frac{N_A\,N_D}{n_i^2} \right) \simeq 0.65 \ \text{ V}. \tag{D.1}$$

21.2 The relations to be used are (21.51), (21.55), and (21.57). If $k_p = 0$, $k_n > 0$, one finds $Y_p = 0$, $Y_n = 1 - \exp\left[-m(b)\right]$. On the other hand it is in this case $m(b) = \int_a^b k_n \,\mathrm{d}x > 0$, whence $Y_n < 1$. If, instead, $k_n = 0$, $k_p > 0$, one finds $Y_n = 0$, $Y_p = 1 - \exp\left[m(b)\right]$ with $m(b) = -\int_a^b k_p \,\mathrm{d}x < 0$, whence $Y_p < 1$. In conclusion, the condition for avalanche never occurs.

Problems of Chap. 22

22.1 The differential capacitance of the MOS structure, extracted from (22.19) and (22.20), reads

$$\frac{C}{C_{\text{ox}}} = \frac{1}{1 + C_{\text{ox}}/C_{\text{sc}}}, \qquad C_{\text{sc}} = \pm \frac{\sqrt{2}\,\varepsilon_{\text{sc}}}{L_A} \frac{\mathrm{d}F}{\mathrm{d}u_s} > 0,$$

where the plus (minus) sign holds for $u_s > 0$ ($u_s < 0$). From (22.3) and (22.5) one finds $\mathrm{d}F^2/\mathrm{d}u_s = A(u_s)$; on the other hand it is $\mathrm{d}F^2/\mathrm{d}u_s = 2\,F\,\mathrm{d}F/\mathrm{d}u_s$, whence

$$C_{\mathrm{sc}} = \pm\frac{\varepsilon_{\mathrm{sc}}}{\sqrt{2}\,L_A}\,\frac{A}{F}, \qquad \frac{C_{\mathrm{ox}}}{C_{\mathrm{sc}}} = \pm\frac{F}{r\,A}, \qquad r = \frac{\varepsilon_{\mathrm{sc}}\,t_{\mathrm{ox}}}{\varepsilon_{\mathrm{ox}}\,\sqrt{2}\,L_A}.$$

Then, the $C(V_G)$ relation is found by eliminating u_s from

$$u'_G = u_s \pm 2\,r\,F, \qquad \frac{C}{C_{\mathrm{ox}}} = \frac{1}{1 \pm F/(r\,A)}.$$

In particular, from (22.26) one finds $C(V'_G = 0) = C_{\mathrm{ox}}/[1 + 1/(\sqrt{2}\,r)]$.

Problems of Chap. 23

23.1 The maximum initial profile is $N(x = 0, t = 0) = 2Q/\sqrt{\pi c_1}$. Remembering (23.26), at the end of the diffusion process the profile has become $N(x, t = t_P) = 2Q\,[\pi(c_1+c_2)]^{-1/2}\times\exp\left[-x^2/(c_1+c_2)\right]$, whence $N(x = 0, t = t_P) = 2Q\,[\pi(c_1+c_2)]^{-1/2}$, with t_P the process duration and $c_2 = 4D\,t_P$. From $N(x = 0, t = t_P) = (2/3)\,N(x = 0, t = 0)$ it follows $1/\sqrt{c_1+c_2} = 2/(3\sqrt{c_1})$, $c_2 = (5/4)\,c_1$ and, finally, $t_P = (5/16)\,(c_1/D) = 5{,}000$ s.

23.2 The initial and final profiles are $N_i(x) = 2\,Q\,\exp(-x^2/c_1)/(\pi c_1)^{1/2}$ and, from (23.26), $N_f(x) = 2\,Q\,\exp[-x^2/(c_1+c_2)]/[\pi(c_1+c_2)]^{1/2}$. Letting $N_f = N_i$ and defining $r = [(c_1+c_2)/c_1]^{1/2}$ and $a^2 = (c_1+c_2)\,c_1/c_2$ yields $r = \exp(x^2/a^2)$, whence $\bar{x} = 10^4 \times a\,(\log r)^{1/2} \simeq 2.68\ \mu$m

23.3 Converting to seconds one finds $t_P = 14{,}400$ s, whence $c_2 = 4\,D\,t_P = 14.4\times10^{-6}\ \mathrm{cm}^2$. Considering that $N(x, t = 0) = 2\,Q\,\exp(-x^2/c_1)/(\pi c_1)^{1/2}$ and, from (23.26), $N(x, t = t_P) = 2\,Q\,\exp[-x^2/(c_1+c_2)]/[\pi\,(c_1+c_2)]^{1/2}$, the ratio sought is $N(x = 0, t = t_P)/N(x = 0, t = 0) = [c_1/(c_1+c_2)]^{1/2} = 0.385$.

23.4 Due to (23.26), the final profile is $N_f = 2\,Q\,\exp[-x^2/(c_1+c_2)]/[\pi(c_1+c_2)]^{1/2}$. From $N(\bar{x}) = N_f(0)$ one has $\exp(-\bar{x}^2/c_1) = [c_1/(c_1+c_2)]^{1/2}$. As a consequence, the position sought is $\bar{x} = [(c_1/2)\,\log(1+c_2/c_1)]^{1/2} = 0.83\ \mu$m.

23.5 Due to (23.26) the final profile is $N_f = 2\,Q\,\exp[-x^2/(c_1+c_2)]/[\pi(c_1+c_2)]^{1/2}$. Let $\alpha = 1.1$. From the condition $N_f(0) = N(x = \alpha\sqrt{c_1})$ one derives $1/[\pi(c_1+c_2)]^{1/2} = \exp(-\alpha^2)/(\pi c_1)^{1/2}$, whence $c_1 = c_2/[\exp(2\alpha^2)-1] = 0.976\times10^{-9}\ \mathrm{cm}^2$.

23.6 Letting $c_2 = 4\,D\,t = 2.4\times10^{-8}\ \mathrm{cm}^2$ and $r = c_2/(c_1+c_2) = 4/7$, one eliminates Q at $x = x_0$ to find $N_1/N_2 = \sqrt{1+r}\,\exp[-r\,x_0^2/(c_1+2\,c_2)]$, whence $x_0 = 10^4 \times [(1/r)\,(c_1+2\,c_2)\,\log(\sqrt{1+r}\,N_2/N_1)]^{1/2} = 4.06\ \mu$m.

23.7 Remembering (C.71) one has $Q = \int_0^\infty N_S\,\mathrm{erfc}(x/\sqrt{c})\,\mathrm{d}x = N_S\sqrt{c/\pi}$, whence $c = 4\,D\,t = \lambda^2$, $t = \lambda^2/(4\,D) = 2.99\times10^{16}\ \mathrm{nm}^2\ \mathrm{s}^{-1} \simeq 5$ min.

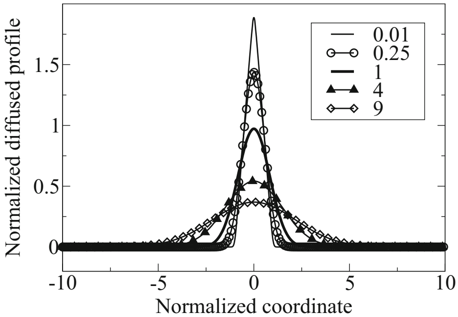


Fig. D.5 Normalized profiles $h\,N/Q$ resulting from the drive-in diffusion of Problem 23.8. The coordinate is $\mu = x/h$. Each profile corresponds to the value of $b(t)$ shown in the legend. The parameter is defined by $b = 4\,a/h^2$, while $a = a(t)$ is defined by the second of (23.10). As explained in Sect. 23.5.2, only the profile's portion on the right of the origin must be considered

23.8 As indicated in Sect. 23.5.2, the initial profile must preliminarily be mirrored onto the negative axis with $N_0 = 2\,Q\,(h + x)/h^2$ for $-h \le x \le 0$ and with $N_0 = 0$ for $x < -h$. Then, the profile is obtained from (23.13) as the portion of $N(x) = (2\,Q/h^2)\,(I^- + I^+)$ calculated for $x \ge 0$, where

$$I^- = \int_{-h}^{0} (h + \xi)\,\Delta(x - \xi, t)\,\mathrm{d}\xi, \qquad I^+ = \int_{0}^{+h} (h - \xi)\,\Delta(x - \xi, t)\,\mathrm{d}\xi$$

and $\Delta(x - \xi, t)$ is given by (C.75). Letting $\eta = (\xi - x)/(4\,a)^{1/2}$, $\mu = x/h$, $b = 4\,a/h^2$, and using (C.66) yields

$$N = (Q/h)\left[(\mu + 1)\,Y^- + (\mu - 1)\,Y^+ - (b/\pi)^{1/2}\,(Z^- + Z^+)\right],$$

with $Y^\mp = \mathrm{erfc}(\mu/\sqrt{b}) - \mathrm{erfc}[(\mu \pm 1)/\sqrt{b}\,]$ and $Z^\mp = \exp\left(-\mu^2/b\right) - \exp\left[-(\mu \pm 1)^2/b\right]$. When $t \to 0^+$ it is $b \to 0$. This makes the $Z^\mp$ terms to vanish, while the terms containing $Y^\mp$ render the initial condition N_0. When $t > 0$ the dose is found by integrating $h\,N$ over μ from 0 to $+\infty$. A somewhat lengthy calculation based on the expressions of Appendix C.7 shows that the integral of $(b/\pi)^{1/2}\,(Z^- + Z^+)$ vanishes whereas that of $(\mu+1)\,Y^- + (\mu-1)\,Y^+$ yields unity. As expected, the result of the dose calculation is Q. The normalized profile $h\,N/Q$ is shown in Fig. D.5 as a function of the normalized coordinate μ at different values of the parameter $b = b(t)$.

Problems of Chap. 24

24.1 The relation between time t and oxide thickness s is given by (24.11), $s^2/c_p + s/c_l = t'$ with $t' = t + s_i^2/c_p + s_i/c_l$. Solving for s and discarding the negative solution yields $s = [(c_p^2/c_l^2 + 4c_p t')^{1/2} - c_p/c_l]/2$, with $c_p/c_l = 0.05\ \mu\mathrm{m}$. It follows $t' = t + s_i^2/c_p + s_i/c_l \simeq 136/60 + 0.995 + 0.237 = 3.50$ h and $4c_p t' = 0.620\ \mu\mathrm{m}^2$.

The total oxide thickness and the thickness of silicon that is consumed in the second process are, respectively, $s = [(0.05^2 + 4c_p t')^{1/2} - 0.05]/2 \simeq 0.369$ μm and $h = 0.44\,(s - s_i) \simeq 70$ nm.

24.2 The gradient sought is found by remembering that, from (24.10), it is $c_p = 2\,w\,k_0\,N_G\,D_O$ and $c_l = w\,k_0\,N_G\,v_r$, whence $c_l/c_p = v_r/(2\,D_O) = 20$ μm^{-1}, $v_r/D_O = 4 \times 10^5$ cm^{-1}. On the other hand, from (24.7,24.6), $-D_O\,\mathrm{grad}N = -D_O\,\mathrm{d}N/\mathrm{d}x = v_r N_I$ whence $\mathrm{d}N/\mathrm{d}x = -N_O\,v_r/D_O = -4 \times 10^{17}$ cm^{-4}.

24.3 Converting the units one finds $c_p = 738$ nm^2 min^{-1}, $c_l = 14.8$ nm min^{-1}. Letting h be the thickness of silicon consumed one has $h = 0.44\,(s - s_i)$, $s = s_i + h/0.44$ whence, from (24.11), $t = (s^2 - s_i^2)/c_p + (s - s_i)/c_l = 150$ min.

24.4 Converting the units yields $c_p = 2000$ nm^2 min^{-1}, $c_l = 50$ nm min^{-1}. From (24.10) it follows $v_r/D_O = 2c_l/c_p = 0.05$, $1 + s\,v_r/D_O = 2$ whence, using (24.8), $N_I = N_O/(1 + s\,v_r/D_O) = 15 \times 10^{11}$ cm^{-3}.

24.5 Converting the units yields $c_p = 11.4$ nm^2 s^{-1}, $c_l = 0.237$ nm s^{-1}. From (24.10) the duration of the first process is found as $t_1 = (s_f^2 - s_i^2)/c_p + (s_f - s_i)/c_l$. Similarly, that of the second process is $t_2 = (s^2 - s_f^2)/c_p + (s - s_f)/c_l$. As the coefficients c_p, c_l are the same one adds the expressions of t_1 and t_2 to each other and lets $s = s_i + \Delta s_1 + \Delta s_2$. This yields $t_1 + t_2 = (s^2 - s_i^2)/c_p + (s - s_i)/c_l = 202$ s.

24.6 Converting the units yields $c_l = 16.67$ nm min^{-1}. Using the definitions (24.10) of c_p and c_l one finds $r = D_O/v_r = c_p/(2\,c_l)$, whence $t_P = [(s^2 - s_i^2)/(2r) + s - s_i]/c_l = 13.9$ min.

24.7 Letting $t = t_P$ and multiplying the first of (24.10) by c_p yields $s^2 + bs + c = 0$ with $b = c_p/c_l$, $c = -s_i^2 - (c_p/c_l)\,s_i - c_p t$. Here s_i and $c_p t_P$ are given while $c_p/c_l = 2D_O/v_r = 2.25 \times 10^{-6}$ cm. Solving for s and discarding the negative root provides the final thickness $s = [(b^2 - 4c)^{1/2} - b]/2 = 76.1$ nm.

24.8 From the relation $\Delta P = s\,\pi r^2\,p_{\mathrm{Si}}$, where ΔP, s are the weight and thickness of the epitaxial layer, and r the wafer's radius, one finds $2\,r = 2\,\sqrt{\Delta P/(\pi s p_{\mathrm{Si}})} \simeq 20.4$ cm $\simeq 8$ in.

24.9 The surface concentration N_S of $SiCl_4$ is found from the relations $s/t = c_l = w\,F_2 = w\,v_r\,N_S$, whence $N_S = s/(w\,v_r\,t) = 1 \times 10^{16}$ cm^{-3}.

24.10 Using $1/w = 5 \times 10^{22}$ cm^{-3} in the relations (24.22,24.23) yields $t = s/c_l = s/(wF_I) = 2$ min.

24.11 Letting t_P be the duration of the process one has, from (24.22,24.23), $c_l = s/t_P = w\,v_r\,N_I$, whence, using 1 μm $= 10^{-4}$ cm, $v_r = s/(w\,N_I\,t_P) = 200$ cm min^{-1}.

24.12 From (24.21) and the second of (24.23) one finds $b = (v_r + v_G)/(v_G\,w\,N_G) = (N_G/N_S)\,(w\,N_G)^{-1} = a/(w\,N_G)$, whence $N_G = a/(w\,b) = 2 \times (5 \times 10^{22}/4.87 \times 10^5) = 2.05 \times 10^{17}$ cm^{-3}.

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