Electrodynamics I — Physics/6111

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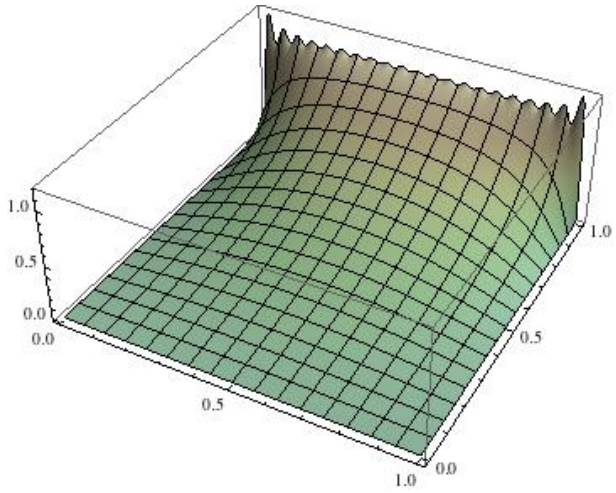

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Chapter 1

Complex Numbers and Calculus

1.1 Motivation

Question: Why do we need complex numbers in physics? Answer: Because they are indispensable for a consistent description of nature.

Example #1: Quantum mechanics of a free particle in one dimension. Hamiltonian operators:

$$H_0 = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,, \qquad p = -\mathrm{i}\hbar\,\frac{\partial}{\partial x}\,. \tag{1.1}$$

Stationary Schrödinger equation:

$$H_0\,\psi(x) = E\psi(x)\,. \tag{1.2}$$

Can solve this through

$$\psi(x) = C\,\exp(\pm kx)\,, \qquad E = -\frac{\hbar^2 k^2}{2m}\,. \tag{1.3}$$

Here, C is a constant. But then we have the problem that the modulus square of the wave function diverges, either for $x \to -\infty$ [if we choose the negative sign in Eq. (1.3)] or for $x \to \infty$ [if we choose the positive sign in Eq. (1.3)]. (The negativity of the energy eigenvalue in Eq. (1.3) is not necessarily a problem, because we could, in principle, define the zero point of the energy anywhere.)

If we want an eigenstate of the Hamiltonian, and a state with a definitive eigenvalue of the momentum, then we need to define a *complex* wave function, proportional to $\exp(\pm\mathrm{i}kx)$,

$$\psi(x) = C\,\exp(\pm\mathrm{i}kx)\,, \qquad p\,\psi(x) = \hbar k\,\psi(x)\,, \qquad E = \frac{\hbar^2 k^2}{2m}\,. \tag{1.4}$$

These wave functions can be normalized to a Dirac-δ, at least, they do not diverge exponentially anywhere on the real axis.

Further Thought: How would the above example have to be generalized to a free particle in three-dimensional space, as opposed to a one-dimensional scenario?

Example #2: Quantum particle with electromagnetic coupling. Let $\vec{A}$ be a vector potential. The Hamiltonian changes into

$$H = \frac{(\vec{p} - q\,\vec{A})^2}{2m}\,, \qquad \vec{p} = -\mathrm{i}\hbar\vec{\nabla}\,. \tag{1.5}$$

Here, q is the charge of the particle.

Reformulate

$$\vec{p} - q\,\vec{A} = -\mathrm{i}\hbar\vec{\nabla} - q\,\vec{A} = -\mathrm{i}\hbar\left(\vec{\nabla} - \mathrm{i}\frac{q}{\hbar}\,\vec{A}\right) = -\mathrm{i}\hbar\vec{\mathcal{D}}\,. \tag{1.6}$$

Here,

$$\vec{\mathcal{D}} = \vec{\nabla} - \mathrm{i}\frac{q}{\hbar}\,\vec{A} \tag{1.7}$$

is the so-called covariant derivative. Without going into detail, we can say that it has the property that the covariant derivative of a gauge-transformed wave function is equal to the gauge transform of the covariant derivative.

The covariant derivative involves a manifestly complex entity in its definition.

In classical electrodynamics, complex numbers are also extremely useful. We will encounter

- Some mathematical techniques like Fourier transformations involves maniestly complex quantities even if the functions to be transformed, are perfectly real.
- Some integrals which we will encounter in the calculation of potentials and fields, are easiest to calculate when we continue the integrand into the complex plane.
- In electrodynamics, is is customary and most appropriate to describe a traveling monochromatic electromagnetic wave with only one Fourier component (rather than two), i.e., using a manifestly complex formalism.
- The so-called Kramers–Kronig relations, which are crucial for a consistent description of the electromagnetic response of media, constitute dispersion relations which manifestly rely on complex numbers.

These are but four examples.

1.2 Modern Gauge Theories and Covariant Coupling

Gauge transformation of the vector potential:

$$\vec{A} \to \vec{A}' = \vec{A} + \vec{\nabla}\Lambda\,. \tag{1.8}$$

Gauge transformed covariant derivative:

$$\vec{\mathcal{D}}' = \vec{\nabla} - \mathrm{i}\frac{q}{\hbar}\,\vec{A}' \tag{1.9}$$

Gauge transformed wave function:

$$\psi' = \exp\left(\frac{\mathrm{i}e\Lambda}{\hbar}\right)\,\psi \tag{1.10}$$

Gauge principle:

$$\begin{aligned}
\vec{\mathcal{D}}'\,\psi' &= \left(\vec{\nabla} - \mathrm{i}\frac{q}{\hbar}\,\vec{A}'\right)\,\psi' \\
&= \left(\vec{\nabla} - \mathrm{i}\frac{q}{\hbar}\,\vec{A} - \mathrm{i}\frac{q}{\hbar}\,\vec{\nabla}\Lambda\right)\,\exp\left(\frac{\mathrm{i}e\Lambda}{\hbar}\right)\,\psi \\
&= \exp\left(\frac{\mathrm{i}e\Lambda}{\hbar}\right)\,\left(\vec{\nabla} - \mathrm{i}\frac{q}{\hbar}\,\vec{A}\right)\,\psi = (\vec{\mathcal{D}}\,\psi)'
\end{aligned} \tag{1.11}$$

The gauge transformed covariant derivative, applied to the gauge transformed wave function, is equal to the the gauge transform of the covariant derivative.

All modern gauge theories rely on this principle: quantum electrodynamics, the electroweak theory, and quantum chromodynamics. Modern physics would be unthinkable without complex numbers.

1.3 Matrix multiplication and complex arithmetic

Recap and Example

A brief recap of matrix multiplication. Take two 2×2 matrices and consider the matrix product.

$$\begin{pmatrix} A & C \\ B & D \end{pmatrix} \begin{pmatrix} E & G \\ F & H \end{pmatrix} = \begin{pmatrix} AE + CF & AG + CH \\ BE + DF & BG + DH \end{pmatrix} \tag{1.12}$$

Entries in the product matrix equal the scalar products of the row vectors of the first matrix and the column vectors of the second matrix.

More systematically

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{pmatrix} \tag{1.13}$$

$$a_{ij} \begin{cases} i \text{ row index} \\ j \text{ column index} \end{cases} \tag{1.14}$$

Generally:

$$c = a \cdot b$$

where a, b and c are $N \times N$ matrices. Fundamental matrix multiplication implies that

$$c_{ij} = \sum_{k=1}^{N} a_{ik} b_{kj} \, . \tag{1.15}$$

Exercise: $N = 2$ and verify consistency with formula (1.15).

1.3.1 Rotation Matrices in Two Dimensions

Consider a matrix of the form

$$R(\vartheta) = \begin{pmatrix} \cos\vartheta & -\sin\vartheta \\ \sin\vartheta & \cos\vartheta \end{pmatrix} \tag{1.16}$$

and let us see how it acts on the vectors

$$\hat{e}_x = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \hat{e}_y = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.17}$$

One obtains

$$R(\vartheta)\cdot\hat{e}_x=\begin{pmatrix}\cos\vartheta & -\sin\vartheta\\ \sin\vartheta & \cos\vartheta\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}\cos\vartheta\\ \sin\vartheta\end{pmatrix} \tag{1.18}$$

We start with $\hat{e}_x$ end with $\cos\vartheta\hat{e}_x+\sin\vartheta\hat{e}_y$: (active) rotation by an angle ϑ.

$$R(\vartheta)\cdot\hat{e}_y=\begin{pmatrix}\cos\vartheta & -\sin\vartheta\\ \sin\vartheta & \cos\vartheta\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}-\sin\vartheta\\ \cos\vartheta\end{pmatrix} \tag{1.19}$$

Here we start with $\hat{e}_y$ end with $-\sin\vartheta\hat{e}_x+\cos\vartheta\hat{e}_y$. Again, (active) rotation by an angle ϑ.

$$\text{paradigm}\quad\begin{cases}\text{matrix multiplication} = \text{rotation operation}\\ \text{matrix} = \text{operator}\end{cases} \tag{1.20}$$

Concatenation of rotation operators

$$R(\vartheta_2)R(\vartheta_1)=\begin{pmatrix}\cos\vartheta_2 & -\sin\vartheta_2\\ \sin\vartheta_2 & \cos\vartheta_2\end{pmatrix}\begin{pmatrix}\cos\vartheta_1 & -\sin\vartheta_1\\ \sin\vartheta_1 & \cos\vartheta_1\end{pmatrix} \tag{1.21}$$

This matrix describes a subsequent rotation by θ_2, following a rotation by θ_1. When acting on vector, the vector first gets rotated by ϑ_1, then by ϑ_2.

One shows that

$$R(\vartheta_2)R(\vartheta_1)=\begin{pmatrix}\cos\vartheta_1\cos\vartheta_2-\sin\vartheta_2\sin\vartheta_1 & -\sin\vartheta_1\cos\vartheta_2-\sin\vartheta_2\cos\vartheta_1\\ \sin\vartheta_2\cos\vartheta_1+\cos\vartheta_2\sin\vartheta_1 & -\sin\vartheta_1\sin\vartheta_2+\cos\vartheta_2\cos\vartheta_1\end{pmatrix}. \tag{1.22}$$

This can be simplified by fundamental trigonometric identities,

$$R(\vartheta_2)R(\vartheta_1)=\begin{pmatrix}\cos(\vartheta_1+\vartheta_2) & -\sin(\vartheta_1+\vartheta_2)\\ \sin(\vartheta_1+\vartheta_2) & \cos(\vartheta_1+\vartheta_2)\end{pmatrix}=R(\vartheta_1+\vartheta_2) \tag{1.23}$$

The geometrical interpretation is now obvious! Rotation by angle ϑ_1, then by ϑ_2, which is the same as a rotation by $\vartheta_1+\vartheta_1$! It is also clear that

$$R(\vartheta_1+\vartheta_2)=R(\vartheta_2+\vartheta_1) \tag{1.24}$$

by elementary geometry. so

$$R(\vartheta_1)R(\vartheta_2)=R(\vartheta_2)R(\vartheta_1) \tag{1.25}$$

or

$$R(\vartheta_1)R(\vartheta_2)-R(\vartheta_2)R(\vartheta_1)=0 \tag{1.26}$$

1.3.2 Commutator of Matrices

$$[a,b]=a\cdot b-b\cdot a \tag{1.27}$$

if a and b were numbers then their commutator would vanish! For rotation matrices this is still true.

$$[R(\vartheta_1),R(\vartheta_2)]=0 \tag{1.28}$$

Note: It does not matter in which sequence the matrices are applied.

1.3.3 Nontriviality of commutators

Consider one rotation matrix

$$R(\vartheta) = \begin{pmatrix} \cos\vartheta & -\sin\vartheta \\ \sin\vartheta & \cos\vartheta \end{pmatrix} \tag{1.29}$$

and a projection matrix

$$\mathbb{P}_x = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{cases} \text{For the geeks:} \\ \text{This is the dyadic product} \\ \hat{e}_x \otimes \hat{e}_x \end{cases} \tag{1.30}$$

How does $\mathbb{P}_x$ act on a vector: $\vec{v} = v_x\hat{e}_x + v_y\hat{e}_y + v_z\hat{e}_z$?

$$\mathbb{P}_x \begin{pmatrix} v_x \\ v_y \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} v_x \\ v_y \end{pmatrix} = \begin{pmatrix} v_x \\ 0 \end{pmatrix} \tag{1.31}$$

Projector property: extraction of x-component

Example

Consider

$$R(\vartheta)\mathbb{P}_x \text{ versus } \mathbb{P}_x R(\vartheta)\,. \tag{1.32}$$

One compares two operations, first, an operation where one projects onto the x axis, then, a rotation by an angle θ, versus an operation where one first rotates by an angle θ, and then projects onto the x axis.

Choose $\vec{v} = \hat{e}_x$ and apply to both matrix products outlined in Eq. (1.32). The first sequences gives:

$$\text{first sequence: } \left\{ R(\vartheta)\mathbb{P}_x \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\vartheta & -\sin\vartheta \\ \sin\vartheta & -\cos\vartheta \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\vartheta \\ \sin\vartheta \end{pmatrix} \right. . \tag{1.33}$$

The second sequences gives:

$$\text{second sequence: } \left\{ \mathbb{P}_x R(\vartheta) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \cos\vartheta \\ \sin\theta \end{pmatrix} = \begin{pmatrix} \cos\vartheta \\ 0 \end{pmatrix} \right. . \tag{1.34}$$

Result:

$$R(\vartheta)\mathbb{P}_x\hat{e}_x \neq \mathbb{P}_x R(\vartheta)\hat{e}_x\,. \tag{1.35}$$

So,

$$[R(\vartheta), \mathbb{P}_x] \neq 0\,. \tag{1.36}$$

The commutator of rotation and projection does not vanish. Geometrically, it is clear that if I rotate first, then project, the result will be different from what I obtain when I project first then rotate. Matrix multiplication is non-commutative!

1.3.4 Matrices and Complex Numbers

Consider a matrix representation of a complex number:

$$\mathbb{M}(z) = \begin{pmatrix} \mathrm{Re}z & -\mathrm{Im}z \\ \mathrm{Im}z & \mathrm{Re}z \end{pmatrix} . \tag{1.37}$$

Then, surprisingly,

$$\begin{aligned}\mathbb{M}(z_1)\mathbb{M}(z_2) &= \begin{pmatrix} \mathrm{Re}z_1 & -\mathrm{Im}z_1 \\ \mathrm{Im}z_1 & \mathrm{Re}z_1 \end{pmatrix} \begin{pmatrix} \mathrm{Re}z_2 & -\mathrm{Im}z_2 \\ \mathrm{Im}z_2 & \mathrm{Re}z_2 \end{pmatrix} \\ &= \begin{pmatrix} \mathrm{Re}z_1\mathrm{Re}z_2 - \mathrm{Im}z_1\mathrm{Im}z_2 & -\mathrm{Re}z_1\mathrm{Im}z_2 - \mathrm{Im}z_1\mathrm{Re}z_2 \\ \mathrm{Im}z_1\mathrm{Re}z_2 - \mathrm{Im}z_2\mathrm{Re}z_1 & \mathrm{Re}z_1\mathrm{Re}z_2 - \mathrm{Im}z_1\mathrm{Im}z_2 \end{pmatrix} \\ &= \mathbb{M}(z_1 \cdot z_2)\,. \end{aligned} \tag{1.38}$$

Here, by $z_1 \cdot z_2$, we denote complex multiplication. Likewise,

$$\mathbb{M}(z_1) + \mathbb{M}(z_2) = \mathbb{M}(z_1 + z_2) \tag{1.39}$$

and

$$\mathbb{M}(z_1/z_2) = \mathbb{M}(z_1)\left[\mathbb{M}(z_2)\right]^{-1} \tag{1.40}$$

The matrix representation of the inverse of a complex matrix is the inverse of the matrix representation of the same complex number! We can also show commutativity,

$$\mathbb{M}(z_1 \cdot z_2) = \mathbb{M}(z_1) \cdot \mathbb{M}(z_2) \tag{1.41}$$

$$= \mathbb{M}(z_2) \cdot \mathbb{M}(z_1) \tag{1.42}$$

$$= \mathbb{M}(z_2 \cdot z_1) \tag{1.43}$$

How can we put the commutativity into context. This is simple,

$$\begin{aligned}\mathbb{M}(z) &= \begin{pmatrix} \mathrm{Re}z & -\mathrm{Im}z \\ \mathrm{Im}z & \mathrm{Re}z \end{pmatrix} \\ &= \sqrt{(\mathrm{Re}z)^2 + (\mathrm{Im}z)^2} \begin{pmatrix} \frac{\mathrm{Re}z}{\sqrt{(\mathrm{Re}z)^2+(\mathrm{Im}z)^2}} & -\frac{\mathrm{Im}z}{\sqrt{(\mathrm{Re}z)^2+(\mathrm{Im}z)^2}} \\ \frac{\mathrm{Im}z}{\sqrt{(\mathrm{Re}z)^2+(\mathrm{Im}z)^2}} & \frac{\mathrm{Re}z}{\sqrt{(\mathrm{Re}z)^2+(\mathrm{Im}z)^2}} \end{pmatrix} \end{aligned} \tag{1.44}$$

The matrix multiplying the complex modulus $|z| = \sqrt{(\mathrm{Re}z)^2 + (\mathrm{Im}z)^2}$ is a rotation matrix if we identify

$$\cos\vartheta = \frac{\mathrm{Re}z}{\sqrt{(\mathrm{Re}z)^2 + (\mathrm{Im}z)^2}} \tag{1.45a}$$

$$\sin\vartheta = \frac{\mathrm{Im}z}{\sqrt{(\mathrm{Re}z)^2 + (\mathrm{Im}z)^2}} \tag{1.45b}$$

We can see that

$$\cos\vartheta^2 + \sin\vartheta^2 = 1 \tag{1.46}$$

So,

$$\mathbb{M}(z) = |z|\ R(\vartheta)\,. \tag{1.47}$$

From our previous considerations on rotation matrices, the property

$$\begin{aligned}\mathbb{M}(z_1)\mathbb{M}(z_2) &= |z_1|\,|z_2|\,R(\vartheta_1 + \vartheta_2) \\ &= \mathbb{M}(z_2)\,\mathbb{M}(z_1)\end{aligned} \tag{1.48}$$

follows. New interpretation of the imaginary unit:

$$\mathbb{M}(\mathrm{i}) = \mathbb{M}(0+\mathrm{i}) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \mathrm{R}(90^\circ) \tag{1.49}$$

Note that the imaginary unit is a rotation by 90 degrees!

$$\mathbb{M}(\mathrm{i})\,\mathbb{M}(\mathrm{i}) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{1.50}$$

$$= -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.51}$$

$$= \mathbb{I}_{2\times 2} = \mathbb{M}(-1) \tag{1.52}$$

The formula $\mathrm{i}^2 = -1$ simply means that a rotation by $90^\circ + 90^\circ = 180^\circ$ inverts (changes sign) of any two-dimensional vector! Likewise,

$$\mathbb{M}(-\mathrm{i}) = \mathbb{M}(0-\mathrm{i}) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathrm{R}(-90^\circ)\,. \tag{1.53}$$

Of course,

$$\mathbb{M}(-\mathrm{i}) \cdot \mathbb{M}(-\mathrm{i}) = \mathbb{M}(-1) \tag{1.54}$$

For Geeks

Geek Aspect #1: We have seen: There is a subset of 2×2 matrices with the structure

$$\begin{pmatrix} \mathrm{Re}z & -\mathrm{Im}z \\ \mathrm{Im}z & \mathrm{Re}z \end{pmatrix} = \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \tag{1.55}$$

which behave as numbers. Important: For two matrices $\mathbb{M}(z_1)$ and $\mathbb{M}(z_2)$ with $z_1 \neq 0$ and $z_2 \neq 0$ we cannot have

$$\mathbb{M}(z_1)\mathbb{M}(z_2) = 0_{2\times 2} \tag{1.56}$$

Why not? Let us assume the contrary and investigate the consequences. Let us assume we can fulfill

$$A \cdot B = 0 \qquad A \neq 0,\, B \neq 0 \tag{1.57}$$

in our algebra, Then

$$A = 0/B \tag{1.58}$$

We found a way to divide zero! Not so good. The algebra of complex numbers is zerodivisor free!

Geek Aspect #2: We can write: Pauli matricies

$$\sigma_x == \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.59}$$

Then, our representation of complex numbers becomes

$$\mathbb{M}(z) = \mathrm{Re}z \cdot \mathbb{I}_{2\times 2} - \mathrm{i}\sigma_y\,\mathrm{Im}z \tag{1.60}$$

The role of the σ_x and σ_z matrices will be discussed later.

Geek Aspect #3: Theorem of Bott and Milnor. There exist zero-divisor-free multiplication algebras only in 1, 2, 4, and 8 dimensions. See *On the parallelizability of the spheres* by R. Bott and J. Milnor, Bull. Amer. Math. Soc. **64**, 87-89 (1958).

1.4 Elementary Calculations: Complex Numbers

1.4.1 Complex Numbers and Trigonometry

Notation:

$$[x, y: \text{ real } ; \ z: \text{ complex}] \tag{1.61}$$

Elementary Euler formula:

$$\mathrm{e}^{\mathrm{i}x} = \cos x + \mathrm{i}\sin x \quad \text{[Euler's Equation]} \tag{1.62a}$$

$$\mathrm{e}^{\mathrm{i}\pi} = -1 \quad \text{[Famous!]} \tag{1.62b}$$

Example #1:

$$\mathrm{e}^{2\mathrm{i}x} = \cos 2x + \mathrm{i}\sin 2x \tag{1.63}$$

Take

$$\begin{aligned} \mathrm{e}^{2\mathrm{i}x} =& \mathrm{e}^{\mathrm{i}x} \cdot \mathrm{e}^{\mathrm{i}x} \\ &= (\cos x + \mathrm{i}\sin x)(\cos x + \mathrm{i}\sin x) \\ &= \cos^2 x - \sin^2 x + \mathrm{i}(2\sin x \cos x) \end{aligned} \tag{1.64}$$

Comparison of the coefficients in Eq.(1.63) and Eq.(1.64) gives

$$\begin{aligned} \cos 2x =& \cos^2 x - \sin^2 x = \text{[Real part]} \\ \sin 2x =& 2\sin x \cos x = \text{[Imaginary part]} \end{aligned} \tag{1.65}$$

Example #2: On one hand,

$$\mathrm{e}^{3\mathrm{i}x} = \cos 3x + \mathrm{i}\sin 3x \tag{1.66}$$

On the other hand,

$$\begin{aligned} \mathrm{e}^{3\mathrm{i}x} &= \mathrm{e}^{\mathrm{i}x} \cdot \mathrm{e}^{\mathrm{i}x} \cdot \mathrm{e}^{\mathrm{i}x} \\ &= (\cos x + \mathrm{i}\sin x)^3 \\ &= \cos^3 x + 3\mathrm{i}\cos^2 x \sin x + 3\mathrm{i}^2 \sin^2 x \cos^2 x + \mathrm{i}^3 \sin^3 x \\ &= \cos^3 x - 3\sin^2 x \cos x + \mathrm{i}\left(3\cos^2 x \sin x - \sin^3 x\right) \end{aligned} \tag{1.67}$$

Comparison of coefficients in Eq. (1.66) and Eq. (1.67) gives

$$\begin{aligned} \cos^3 x =& \cos^3 x - 3\sin^2 x \cos x = \text{[Real part]} \\ \sin 3x =& 3\cos x \sin x - \sin^3 x = \text{[Imaginary part]} \end{aligned} \tag{1.68}$$

1.4.2 Functions of a Complex Variable

Example #1:

$$f(z) = \mathrm{e}^{z} = \mathrm{e}^{x}\mathrm{e}^{\mathrm{i}y} = \mathrm{e}^{x}\left(\cos y + \mathrm{i}\sin y\right) = \mathrm{e}^{x}\cos y + \mathrm{i}\mathrm{e}^{x}\sin y \tag{1.69a}$$

Example #2:

$$f(z) = \mathrm{e}^{\mathrm{i}z} = \mathrm{e}^{\mathrm{i}x}\mathrm{e}^{-y} = \mathrm{e}^{y}\cos x + \mathrm{i}\mathrm{e}^{-y}\sin x \tag{1.69b}$$

Example #3:

$$\begin{aligned} f(z) = z^3 = (x+\mathrm{i}y)^3 = x^3 + 3\mathrm{i}x^2y + 3x^2y^2 + \mathrm{i}^3y^3 \\ x^3 - 3\mathrm{i}xy^2 + \mathrm{i}\left(3x^2y - y^3\right) \end{aligned} \tag{1.70}$$

Example #4:

$$f(z) = z^2 = (x+\mathrm{i}y)^2 = \ x^2 - y^2 + \mathrm{i}2xy\,. \tag{1.71}$$

1.4.3 Partial Derivatives and Strange Observations

Now, let's record some observations. General identification:

$$f(z) = f_1(x,y) + \mathrm{i}f_2(x,y) \tag{1.72}$$

Start with the complex function,

$$f(z) = z^2 \tag{1.73}$$

Separating the real and imaginary parts gives,

$$f_1(x,y) = x^2 - y^2 \tag{1.74a}$$

$$f_2(x,y) = 2xy \tag{1.74b}$$

We now take the partial derivatives of both functions, **[for an orientation on partial derivatives, see Figs. 1.1 and 1.2]**

$$\frac{\partial f_1}{\partial x} - \frac{\partial f_2}{\partial y} = (2x) - (2x) = 0 \tag{1.75a}$$

$$\frac{\partial f_2}{\partial x} + \frac{\partial f_1}{\partial y} = (2y) + (-2y) = 0 \tag{1.75b}$$

Example #2: Again, start with the complex function,

$$f(z) = z^3\,. \tag{1.76}$$

Separating the real and imaginary parts gives,

$$f_1(x,y) = x^3 - 3xy^2 \tag{1.77a}$$

and

$$f_2(x,y) = 3x^2y - y^3 \tag{1.77b}$$

We now take the partial derivatives of both functions,

$$\left.\begin{aligned}\frac{\partial f_2}{\partial y} &= 3x^2 - 3y^2 \\ \\ \frac{\partial f_1}{\partial x} &= 3x^2 - 3y^2\end{aligned}\right\} \text{same!} \tag{1.78a}$$

Also,

$$\left.\begin{aligned}\frac{\partial f_1}{\partial y} &= -6xy \\ \\ \frac{\partial f_2}{\partial x} &= 6xy\end{aligned}\right\} \text{opposite!} \tag{1.78b}$$

Thus, for all functions of z we have examined, we find

$$\frac{\partial f_1}{\partial x} - \frac{\partial f_2}{\partial y} = 0\,, \tag{1.79a}$$

$$\frac{\partial f_2}{\partial x} + \frac{\partial f_1}{\partial y} = 0 \tag{1.79b}$$

Strange! We will need to find an explanation. It comes from the Cauchy–Riemann equations.

1.5 Complex Numbers and Vector Fields

1.5.1 Outline

Explanation Requires Further Study

We have to get familiar with:

- Partial Derivatives
- Complex Contour Integration
- Divergence Theorem and Stokes Theorem $(2D)$
- Chain Rule for Partial Derivatives.

Let us go step by step.

1.5.2 Definition of Vector Field

Local elevation on a mountain: function $h = h(x, y)$. See Figs. 1.1 and 1.2. Now. Have vector field. Connection of height to $2D$ vector field. Two "h" functions F_x and F_y each multiplying a unit vector, $\hat{e}_x$ and $\hat{e}_y$

$$\vec{F}(x, y) = F_x(x, y)\hat{e}_x + F_y(x, y)\hat{e}_y \tag{1.80}$$

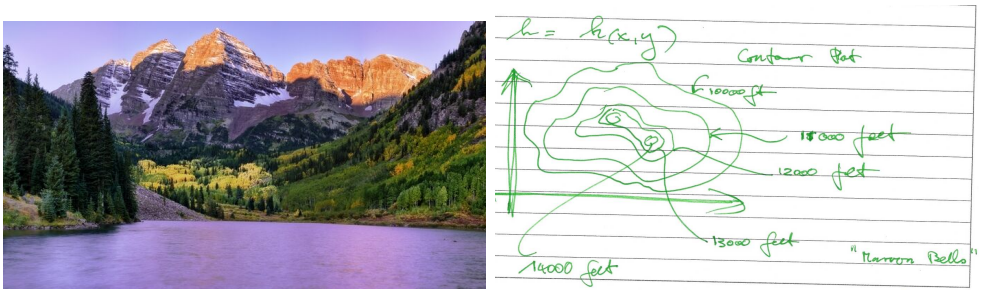

Figure 1.1: Approximate topological map of Maroon Bells, showing change in elevation. Lines represent equal altitude.

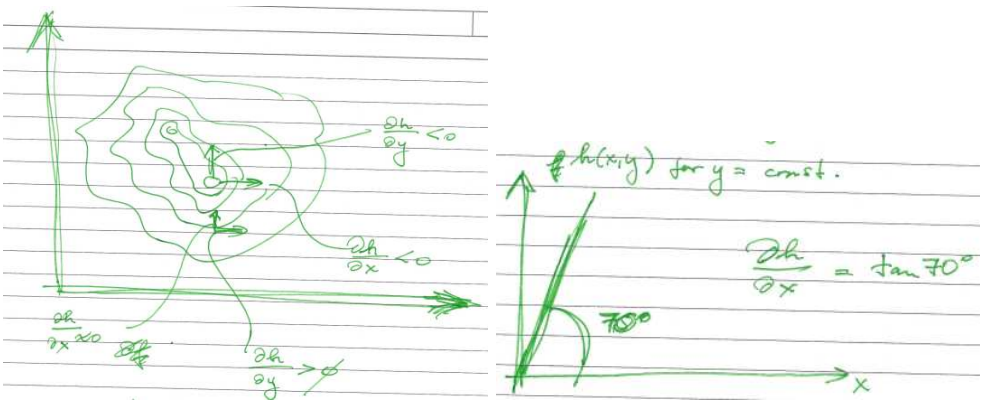

Figure 1.2: Change in height in the x and y directions represented using partial derivatives. Also, conversion of a derivative into an angle.

Example:

$$F_x = \frac{x}{x^2+y^2} \qquad\qquad F_y = \frac{y}{x^2+y^2} \tag{1.81}$$

1.5.3 Definition of Complex Contour Integral

The definition of a contour integral implies that

$$I = \int_C f(z)\mathrm{d}z = \int_{t_1}^{t_2} f(z(t))\frac{\mathrm{d}z(t)}{\mathrm{d}t}\,\mathrm{d}t\,. \tag{1.82}$$

Here, one assumes that $z(t_1) = z_1$ is the start point of the contour, while $z(t_2) = z_2$ is the end point of the contour. The parameterization $z = z(t)$ has to be chosen so that it goes along the contour C.

Now, let us think about the contour C as a river (say, the meandering Gasconade) and about the parameterization $z(t)$ as the position of a kayaker at time t. Let us alzo consider that a different kayaker will pass the same points on the Gasconade at a different time s, possibly, with a different start time s_1 and a different end time s_2. Now, since the two kayakers are going on the same river, they still need to pass every point on the river once. There must thus be a mapping $t = t(s)$ which maps the time s at which the second kayaker passed a given point, against the time t where the first kayaker passed the same point.

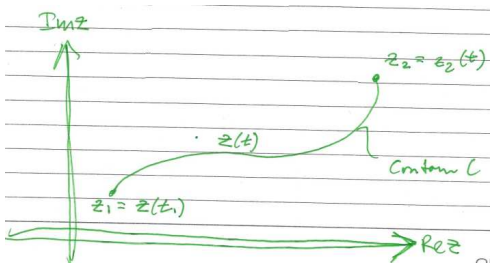

Figure 1.3: When is the contour integral independent of the actual contour and only dependent on the start and end points z_1 and z_2?

Our task is to investigate whether or not the function

$$\tilde{z}(s) = (z \odot t)(s) = z(t(s)) \tag{1.83}$$

is another valid parameterization of the contour, and whether or not the representation (1.82) remains valid. With the help of the relation (chain rule)

$$\frac{\mathrm{d}z(t(s))}{\mathrm{d}s} = \left.\frac{\mathrm{d}z}{\mathrm{d}t}\right|_{t=(t(s)} \frac{\mathrm{d}t(s)}{\mathrm{d}s}\,, \tag{1.84}$$

one has

$$\begin{aligned}
\tilde{I} &= \int_{s_1}^{s_2} f(\tilde{z}(s)) \frac{\mathrm{d}\tilde{z}(s)}{\mathrm{d}s}\,\mathrm{d}s \\
&= \int_{s_1}^{s_2} f(z(t(s))) \frac{\mathrm{d}z(t(s))}{\mathrm{d}s}\,\mathrm{d}s \\
&= \int_{s_1}^{s_2} f(z(t(s)))\, \left.\frac{\mathrm{d}z}{\mathrm{d}t}\right|_{t=(t(s)} \frac{\mathrm{d}t(s)}{\mathrm{d}s}\mathrm{d}s \\
&= \int_{t_1}^{t_2} f(z(t)) \frac{\mathrm{d}z(t)}{\mathrm{d}t}\,\mathrm{d}t = I\,.
\end{aligned} \tag{1.85}$$

This shows the reparameterization invariance of a contour integral.

1.5.4 Complex Contour Integration and Vector Fields

Fundamental relation:

$$\begin{aligned}
\int\limits_C f(z)\mathrm{d}z &= \int_{t_1}^{t_2} f(z(t)) \frac{\mathrm{d}z(t)}{\partial t}\mathrm{d}t \\
&= \int \left[f_1(x,y) + \mathrm{i}f_2(x,y)\right] \left(\frac{\partial x(t)}{\partial t} + \mathrm{i}\frac{\partial y(t)}{\partial t}\right) \mathrm{d}t \\
&= \int \left(f_1(x,y)\frac{\partial x(t)}{\partial t} - f_2(x,y)\frac{\partial y(t)}{\partial t}\right) \mathrm{d}t \\
&\quad + \mathrm{i}\int \left(f_2(x,y)\frac{\partial x(t)}{\partial t} + f_1(x,y)\frac{\partial y(t)}{\partial t}\right) \mathrm{d}t
\end{aligned} \tag{1.86}$$

When is the contour integral in Fig. 1.5.1 independent of the actual contour and only dependent on the start and end points z_1 and z_2?

We start by looking at the connection between the following equations,

$$f(z) = f_1(z) + \mathrm{i}f_2(z) = f_1(x,y) + \mathrm{i}f_2(x,y) \tag{1.87a}$$

and the vector fields

$$\vec{F}(x,y) = f_1(x,y)\hat{e}_x + f_2(x,y)\hat{e}_y \qquad \vec{F}^*(x,y) = f_1(x,y)\hat{e}_x - f_2(x,y)\hat{e}_y \tag{1.87b}$$

Can find a connection between complex contour integration and vector fields. Have

$$\begin{aligned}
\int f(z)\mathrm{d}z &= \int (f_1(z) + \mathrm{i}f_2(z)) \left(\frac{\partial x_1}{\partial t} + \mathrm{i}\frac{\partial x_2}{\partial t} \right) \mathrm{d}t \\
&= \int \left[f_1(z)\frac{\partial x_1}{\partial t} - f_2(z)\frac{\partial x_2}{\partial t} \right] \mathrm{d}t \\
&\quad + \mathrm{i} \left[f_2(t)\frac{\partial x_1}{\partial t} + f_1(z)\frac{\partial x_2}{\partial t} \right] \mathrm{d}t \\
&= \int (f_1(x,y)\hat{e}_x - f_2(x,y)\hat{e}_y) \underbrace{\left(\hat{e}_x \frac{\partial x_1}{\partial t} + \hat{e}_y \frac{\partial x_2}{\partial t} \right) \mathrm{d}t}_{=\mathrm{d}\vec{\ell}} \\
&\quad + \mathrm{i} \int (f_2(x,y)\hat{e}_x + f_1(x,y)\hat{e}_y) \underbrace{\left(\hat{e}_x \frac{\partial x_1}{\partial t} + \hat{e}_y \frac{\partial x_2}{\partial t} \right) \mathrm{d}t}_{=\mathrm{d}\vec{\ell}} \\
&= \int \vec{F}^* \cdot \mathrm{d}\vec{\ell} + \mathrm{i} \int (\hat{e}_z \times \vec{F}^*) \cdot \mathrm{d}\vec{\ell}
\end{aligned} \tag{1.88}$$

Infinitesimal element along the complex path in the complex plane is $\mathrm{d}\vec{\ell}$. We found a connection of complex contour integration, and line integrals of two-dimensional vector fields. This motivates us to study two-dimensional vector fields in more detail.

1.6 Basics of the Gradient Operator

1.6.1 Definition

The gradient operator is a vector-valued operator of the form

$$\vec{\nabla} = \hat{e}_x \frac{\partial}{\partial x} + \hat{e}_y \frac{\partial}{\partial y} \tag{1.89}$$

It is important to note that,

$$\vec{\nabla} \neq \nabla_x + \nabla_y\,, \qquad \vec{\nabla} \neq \vec{\nabla}_x \cdot \vec{\nabla}_y \tag{1.90}$$

The vector $\vec{\nabla}$ is a vector, because it has x and y components, and because of the presence of unit operators $\hat{e}_x$ and $\hat{e}_y$. It is an operator due to the presence of the partial derivatives $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$.

$$\vec{\nabla} f = (\vec{\nabla} f) \tag{1.91}$$

Input: Scalar function. Output: Vector field.

$$\vec{\nabla} \cdot \vec{F} = (\vec{\nabla} \cdot \vec{F}) \tag{1.92}$$

Input: vector valued function Output: scalar function

$$\left(\vec{\nabla} \times \vec{F}\right)_z = \frac{\partial}{\partial x} F_y \frac{\partial}{\partial y} F_x \tag{1.93}$$

The curl has only one componene in "2D"

1.6.2 Poisson Equation, Potentials and Vector Fields

The Poisson equation is defined as

$$\vec{\nabla}^2 f(x, y) = 0\,. \tag{1.94}$$

Define the gradient of a function f which fulfills the Poisson equation:

$$\vec{F}(x, y) = \vec{\nabla} f(x, y) = (\vec{\nabla} f)(x, y) \tag{1.95}$$

Calculate:

$$\begin{aligned} \left(\vec{\nabla} \times \vec{F}\right)_z &= \frac{\partial}{\partial x}\frac{\partial}{\partial y} f - \frac{\partial}{\partial y}\frac{\partial}{\partial x} f && (1.96)\\ &= \left(\vec{\nabla} \times \vec{\nabla} f\right)_z && (1.97)\\ &= \left(\vec{\nabla} \times \vec{\nabla}\right) f = 0 && (1.98) \end{aligned}$$

By assumption (Poisson equation)

$$\left(\vec{\nabla} \cdot \vec{F}\right) = \vec{\nabla}^2 f = 0 \tag{1.99}$$

General result: If

$$\vec{\nabla}^2 f = 0 \tag{1.100}$$

then we can define a divergence and curl-free vector field by the relation

$$\vec{F} = \vec{\nabla} f \tag{1.101}$$

One possible interpretation of our observations is as follows [see Eq. (1.87b)]:

$$\frac{\partial f_1}{\partial x} - \frac{\partial f_2}{\partial y} = 0 \qquad \Leftrightarrow \qquad \vec{\nabla} \cdot \vec{F}^* = 0\,, \tag{1.102a}$$

$$\frac{\partial f_2}{\partial x} + \frac{\partial f_1}{\partial y} = 0 \qquad \Leftrightarrow \qquad \left(\vec{\nabla} \times \vec{F}^*\right)_z = 0\,, \tag{1.102b}$$

We experimentally observe that complex functions are accompanied by a divergence-free, and curl-free, vector field $\vec{F}^*$. But that is just a reformulation of our observations, not an explanation!

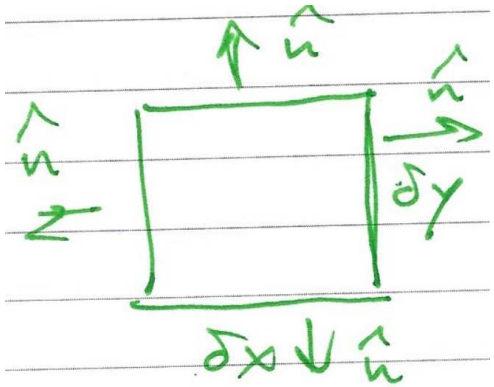

Figure 1.4: Infinitesimally small rectangle.

1.6.3 Divergence and Stokes's Theorem

Statements. Divergence Theorem. In 2D.

$$\int_A \vec{\nabla} \cdot \vec{F} \mathrm{d}A = \int_{\partial A} \vec{F} \cdot \mathrm{d}\vec{\ell}_\perp \tag{1.103a}$$

Divergence Theorem. In 3D.

$$\int_V \vec{\nabla} \cdot \vec{F} \mathrm{d}V = \int_{\partial V} \vec{F} \cdot \mathrm{d}\vec{A} \tag{1.103b}$$

Stokes's Theorem. In 2D.

$$\int_A \left(\vec{\nabla} \times \vec{F}\right)_z \mathrm{d}A = \int_{\partial A} \vec{F} \cdot \mathrm{d}\vec{\ell} \tag{1.104a}$$

Stokes's Theorem. In 3D.

$$\int_{\partial A} \left(\vec{\nabla} \times \vec{F}\right) \cdot \mathrm{d}\vec{A} = \int_{\partial A} \vec{F} \cdot \mathrm{d}\vec{\ell} \tag{1.104b}$$

Our identification of complex contour integrals with line integrals could suggest to look at Stokes's theorem, which concerns line integrals.

1.6.4 Proof of Divergence Theorem

Consider a (small) rectangle of the form in Fig. (1.4),

$$\begin{aligned}\int_{\partial(\delta A)} \vec{F} \cdot \mathrm{d}\vec{\ell}_\perp =& F_x\left(x+\delta x, y+\frac{1}{2}\delta y\right)\delta y + F_y\left(x+\frac{1}{2}\delta x, y+\delta y\right)\delta x \\ &- F_x\left(x, y+\frac{1}{2}\delta y\right)\delta y - F_y\left(x+\frac{1}{2}\delta x, y\right)\delta x \\ &\approx \frac{\partial F_x}{\partial x}\delta x\delta y + \frac{\partial F}{\partial y} y\delta x\delta y \approx \int_{\delta A}\left(\vec{\nabla}\cdot\vec{F}\right)\mathrm{d}(\delta A)\end{aligned} \tag{1.105}$$

1.6.5 Proof of Stokes's Theorem

Consider the same rectangle but the line elements $\mathrm{d}\vec{\ell}$ along the path:

$$\begin{aligned}\int\limits_{\partial(\delta A)} \vec{F}\cdot\mathrm{d}\vec{\ell} =& F_x\left(x+\frac{\delta x}{2},y\right)\delta x + F_y\left(x+\delta x, y+\frac{1}{2}\delta y\right)\delta y \\ &- F_x\left(x+\frac{\delta x}{2},y+\delta y\right)\delta x - F_y\left(x,y+\frac{1}{2}\delta y\right)\delta y \\ =& -\frac{\partial}{\partial y}F_x\delta x\delta y + \frac{\partial}{\partial x}F_y\delta x\delta y \\ =& \left(\frac{\partial}{\partial x}F_y - \frac{\partial}{\partial y}F_x\right)\delta x\delta y \\ =& \left(\vec{\nabla}\times\vec{F}\right)_z\delta x\delta y \approx \int\limits_{\delta A}\left(\vec{\nabla}\times\vec{F}\right)_z\delta x\delta y\end{aligned} \tag{1.106}$$

Hence, again, by the Lego principle, we can show that, for macroscopic areas, we can define the closed contour integral as,

$$\oint\limits_{\partial A}\vec{F}\cdot\mathrm{d}\vec{\ell} = \int\limits_{A}\left(\vec{\nabla}\times\vec{F}\right)_z\mathrm{d}A \tag{1.107}$$

1.7 Cauchy–Riemann Equations

1.7.1 Dependence on Complex Conjugate

Consider

$$f(z)=f(x,y)\,,\qquad f(z)=f(z,z^*)\,,\qquad x=\frac{z+z^*}{2}\quad y=\frac{z-z^*}{2\mathrm{i}} \tag{1.108}$$

However, the functions we have been considering only depend on z, not z^*. Hence, they must implement some further structure. Let us see: Chain rule says that

$$\frac{\partial}{\partial z^*}=\frac{\partial x}{\partial z^*}\frac{\partial}{\partial x}+\frac{\partial y}{\partial z^*}\frac{\partial}{\partial y}=\frac{1}{2}\frac{\partial}{\partial x}+\frac{\mathrm{i}}{2}\frac{\partial}{\partial y} \tag{1.109}$$

Let us try out:

$$\begin{aligned}\frac{\partial}{\partial z^*}f(z) =& \left(\frac{1}{2}\frac{\partial}{\partial x}+\frac{\mathrm{i}}{2}\frac{\partial}{\partial y}\right)(f_1(x,y)+\mathrm{i}f_2(x,y)) \\ =& \frac{1}{2}\left(\frac{\partial f_1}{\partial x}-\frac{\partial f_2}{\partial y}\right)+\frac{\mathrm{i}}{2}\left(\frac{\partial f_2}{\partial x}+\frac{\partial f_1}{\partial y}\right)\end{aligned} \tag{1.110}$$

If we demand that $f=f(z)$ be a function of z only, not of z^*, then our strange observations recorded in Eq. (1.79) simply say that the functions $f(z)$ do not depend on z^*! We recall that Eq. (1.79) says that

$$\frac{\partial f_1}{\partial x}-\frac{\partial f_2}{\partial y}=0\,,\qquad \frac{\partial f_2}{\partial x}+\frac{\partial f_1}{\partial y}=0\,. \tag{1.111}$$

Also, the derivative with respect to z can be written as

$$\frac{\partial}{\partial z}=\frac{\partial x}{\partial z}\frac{\partial}{\partial x}+\frac{\partial y}{\partial z}\frac{\partial}{\partial y}=\frac{1}{2}\frac{\partial}{\partial x}-\frac{\mathrm{i}}{2}\frac{\partial}{\partial y} \tag{1.112}$$

Hence, we can write

$$\frac{\partial}{\partial z} f(z) = \left(\frac{1}{2} \frac{\partial}{\partial x} - \frac{\mathrm{i}}{2} \frac{\partial}{\partial y} \right) (f_1(x,y) + \mathrm{i} f_2(x,y)) \\ = \frac{1}{2} \left(\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} \right) + \frac{\mathrm{i}}{2} \left(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y} \right) \tag{1.113}$$

The value of the complex derivative cannot depend on the direction in the complex plane we are taking. Hence, in the definition of the partial derivative, we can set

$$\delta z = \delta x \,, \qquad \frac{\mathrm{d}f(z)}{\mathrm{d}z} = \lim_{\delta x \to 0} \frac{f(x + \delta x + \mathrm{i}y) - f(x + \mathrm{i}y)}{\delta x} = \frac{\partial f(z)}{\mathrm{d}x} = \frac{\partial f_1}{\partial x} + \mathrm{i} \frac{\partial f_2}{\partial x} \,. \tag{1.114}$$

A comparison of Eqs. (1.113) and (1.114) reveals that

$$\frac{\partial f_1}{\partial x} = \frac{1}{2} \left(\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} \right) , \qquad \mathrm{i} \frac{\partial f_2}{\partial x} = \frac{\mathrm{i}}{2} \left(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y} \right) \tag{1.115}$$

These two equations can be recast into the form given in Eq. (1.111).

Likewise, we can perform the calculation of the complex derivative by considering an infinitesimal change of the complex argument in the imaginary direction,

$$\delta z = \mathrm{i} \delta y \,, \qquad \frac{\mathrm{d}f(z)}{\mathrm{d}z} = \lim_{\delta y \to 0} \frac{f(x + \mathrm{i}y + \mathrm{i}\delta y) - f(x + \mathrm{i}y)}{\mathrm{i}\delta y} = -\mathrm{i} \frac{\partial f(z)}{\mathrm{d}y} = -\mathrm{i} \frac{\partial f_1}{\partial y} + \frac{\partial f_2}{\partial y} \,. \tag{1.116}$$

The resulting equations, obtained by comparing Eqs. (1.113) and (1.116),

$$\frac{\partial f_2}{\partial y} = \frac{1}{2} \left(\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} \right) , \qquad -\mathrm{i} \frac{\partial f_1}{\partial y} = \frac{\mathrm{i}}{2} \left(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y} \right) , \tag{1.117}$$

and again equivalent to Eq. (1.111).

1.7.2 Corollary and Cauchy–Riemann

From the independence of the function $f(z)$ on z^*, we have thus derived the Cauchy–Riemann relations

$$\frac{\partial f_1}{\partial x} - \frac{\partial f_2}{\partial x} = 0 \,, \qquad \frac{\partial f_2}{\partial x} + \frac{\partial f_1}{\partial y} = 0 \,, \tag{1.118a}$$

These exactly correspond to our strange observations. With Eq. (1.87b), we conclude that the first of these equations can be written as

$$\vec{\nabla} \cdot \vec{F}^* = -[\vec{\nabla} \times (\vec{F}^* \times \hat{e}_z)]_z = 0 \tag{1.118b}$$

The second equation can be written as

$$-[\vec{\nabla} \times \vec{F}^*]_z = 0 \tag{1.118c}$$

So, we confirm that our "strange observations" imply that $\vec{F}^*$ is a divergence and curl-free vector field. We have used the relation

$$\vec{F}^* \times \hat{e}_z = (f_1 \, \hat{e}_x - f_2 \, \hat{e}_y) \times \hat{e}_z = f_1 \, \hat{e}_x \times \hat{e}_z - f_2 \hat{e}_y \times \hat{e}_z = -f_1 \, \hat{e}_y - f_2 \, \hat{e}_x \tag{1.119}$$

which implies that

$$\left[\vec{\nabla} \times (\vec{F}^* \times \hat{e}_z) \right]_z = \left[\vec{\nabla} \times (-f_2 \, \hat{e}_x - f_1 \, \hat{e}_y) \right]_z = -\frac{\partial}{\partial x} f_1 + \frac{\partial}{\partial Y} f_2 = \vec{\nabla} \cdot \vec{F}^* \tag{1.120}$$

Furthermore, of course,

$$\vec{\nabla} \times F^* = \vec{\nabla} \times (f_1\,\hat{e}_x - f_2\,\hat{e}_y) = -\frac{\partial}{\partial x} f_2 - \frac{\partial}{\partial y} f_1\,. \tag{1.121}$$

The complex contour integral along a closed contour is

$$\begin{aligned}
\oint f(z)\mathrm{d}z = & \oint (f_1 + \mathrm{i} f_2)(\mathrm{d}x + \mathrm{i}\mathrm{d}y) \\
= & \oint (f_1 \mathrm{d}x - f_2 \mathrm{d}y) + \mathrm{i} \oint (f_2 \mathrm{d}x + f_1 \mathrm{d}y) \\
= & \int_{\partial A} \vec{F}^* \cdot \mathrm{d}\vec{\ell} - \mathrm{i} \int_{\partial A} [\, \vec{F}^* \times \hat{e}_z \,]_z \cdot \mathrm{d}\vec{\ell} \\
= & \int_A (\vec{\nabla} \times \vec{F}^*)_z \mathrm{d}A - \mathrm{i} \int_A [\, \vec{\nabla} \times (\vec{F}^* \times \hat{e}_z) \,]_z \mathrm{d}A \\
= & \int_A (\vec{\nabla} \times \vec{F}^*)_z \mathrm{d}A + \mathrm{i} \int_A \vec{\nabla} \cdot \vec{F}^* \mathrm{d}A
\end{aligned} \tag{1.122}$$

We have transformed the closed complex contour, which is the basis of the closed-contour integral $\oint$, into a line integral in the mathematically positive direction, surrounding the area A. In general, we can say that area integrals in the last line of Eq. (1.122) vanish in view of Eq. (1.118). This statement does not hold if there are problematic points inside the contour, i.e., if the terms $(\vec{\nabla} \times \vec{F}^*)_z$ and $\vec{\nabla} \cdot \vec{F}^*$ have singularities inside the area A. Interpretation: The relation

$$-\left[\vec{\nabla} \times \vec{F}^*\right]_z = 0 \quad \Leftrightarrow \quad \frac{\partial f_2}{\partial x} + \frac{\partial f_1}{\partial y} = 0\,, \tag{1.123}$$

ensures that the real part of a closed contour integral (1.122) vanishes. The real part of a complex contour integral thus only depends on the start and end point of the contour. The relation

$$\vec{\nabla} \cdot \vec{F}^* = -[\, \vec{\nabla} \times (\vec{F}^* \times \hat{e}_z) \,]_z = 0 \quad \Leftrightarrow \quad \frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} = 0\,, \tag{1.124}$$

ensures that the imaginary part of a contour integral only depends on the start and end point of the contour. It is independent of the path.

We have uncovered an intimate connection between complex functions of a complex variable, curl-free and divergence-free two-dimensional vector fields, Stokes's theorem, and the path independence of complex contour integrals.

In short, the independence of $f(z)$ on z^* ensures that the Cauchy–Riemann conditions hold. These conditions are tantamount to sayting that $\vec{F}^*$ is divergence-free, and curl-free. Yet, since $\vec{F}^*$ is divergence-free, and curl-free, and because we can map complex contour integrals onto line integrals and use Stokes's theorem, we can show that complex contour integrals are path independent and depend only on the start and end point of a complex trajectory.

All of these statements only hold if all relevant vector fields are well-behaved inside the closed contour, which means that they must be analytic. We will come to this point later.

1.7.3 Line Integrals and Divergence Theorem

A geometric consideration reveals that, in two dimensions, for areas enclosed in the mathematically positive sense, there is actually a relation between the infinitesimal line element $\mathrm{d}\ell$ and the perpendicular line element

$\mathrm{d}\ell_\perp$, in the form

$$\mathrm{d}\vec{\ell}_\perp = \mathrm{d}\vec{\ell} \times \hat{e}_z \,. \tag{1.125}$$

Hence, we can alternatively explain the emergence of the divergence $\vec{\nabla} \cdot \vec{F}^*$ in Eq. (1.122) as follows,

$$\begin{aligned}
\oint f(z)\mathrm{d}z &= \oint (f_1 + \mathrm{i}f_2)(\mathrm{d}x + \mathrm{i}\mathrm{d}y) \\
&= \oint (f_1 \mathrm{d}x - f_2 \mathrm{d}y) + \mathrm{i} \oint (f_2 \mathrm{d}x + f_1 \mathrm{d}y) \\
&= \int_{\partial A} \vec{F}^* \cdot \mathrm{d}\vec{\ell} - \mathrm{i} \int_{\partial A} [\, \vec{F}^* \times \hat{e}_z \,]_z \cdot \mathrm{d}\vec{\ell} \\
&= \int_{\partial A} \vec{F}^* \cdot \mathrm{d}\vec{\ell} + \mathrm{i} \int_{\partial A} \vec{F}^* \cdot (\mathrm{d}\vec{\ell} \times \hat{e}_z) \\
&= \int_A (\vec{\nabla} \times \vec{F}^*)_z \mathrm{d}A + \mathrm{i} \int_A \vec{F}^* \cdot \mathrm{d}\vec{\ell}_\perp \\
&= \int_A (\vec{\nabla} \times \vec{F}^*)_z \mathrm{d}A + \mathrm{i} \int_A \vec{\nabla} \cdot \vec{F}^* \mathrm{d}A \,.
\end{aligned} \tag{1.126}$$

The result is the same as in Eq. (1.122) and illustrates the connections between curl and divergence in two dimensions.

1.7.4 Function 1/z

For the vector field $\vec{F}^*$ belonging to the function $f(z) = 1/z$, we had found that is not divergence-free, but probably curl-free. The last statement should be taken with a grain of salt because we actually cannot calculate the curl of $\vec{F}^*$ at the origin, but the field simply does not look like it has a curl. Because the divergence of $\vec{F}^*$ regulates the path independence of the imaginary part of a contour integral, we anticipate that the imaginary part of a closed-contour integral of $1/z$, around the origin, probably has a nonvanishing value. This assumption will be verified in the following.

First, we observe that

$$\begin{aligned}
f(z) = \frac{1}{z} = \frac{z^*}{|z|^2} &= \frac{x - \mathrm{i}y}{x^2 + y^2} \\
&= \frac{x}{x^2 + y^2} - \frac{\mathrm{i}y}{x^2 + y^2} \\
&= \frac{\partial}{\partial x} \ln\left(\frac{\sqrt{x^2 + y^2}}{a}\right) - \mathrm{i} \frac{\partial}{\partial y} \ln\left(\frac{\sqrt{x^2 + y^2}}{a}\right)
\end{aligned} \tag{1.127}$$

This means that the function $f(z) = 1/z$ is associated with the vector field

$$\vec{F}^*(x, y) = \hat{\mathrm{e}}_x \frac{\partial}{\partial x} \ln\left(\frac{\sqrt{x^2 + y^2}}{a}\right) + \hat{\mathrm{e}}_y \frac{\partial}{\partial y} \ln\left(\frac{\sqrt{x^2 + y^2}}{a}\right) = \vec{\nabla} \ln\left(\frac{|\vec{r}|_{D=2}}{a}\right) , \tag{1.128}$$

where $|\vec{r}|_{D=2} = \sqrt{x^2 + y^2}$ is the norm of the position vector in two dimensions. Because F^* is the gradient of a scalar function, one has

$$\vec{\nabla} \times \vec{F}^*(x, y) = \vec{0} \,. \tag{1.129}$$

Recognizing the Green function of the two-dimensional Poisson equation, we have

$$\vec{\nabla}^{\,2} \ln\left(\frac{|\vec{r}|_{D=2}}{a}\right) = \vec{\nabla}^{\,2} \ln\left(\frac{\sqrt{x^2+y^2}}{a}\right) = \frac{\partial^2}{\partial x^2} \ln\left(\frac{\sqrt{x^2+y^2}}{a}\right) + \frac{\partial^2}{\partial y^2} \ln\left(\frac{\sqrt{x^2+y^2}}{a}\right)$$
$$= 2\pi\, \delta^{(2)}(x,y) = 2\pi\, \delta^{(2)}(\vec{r}_{D=2})\,. \tag{1.130}$$

Now, from Eq. (1.126), it follows that

$$\oint f(z)\mathrm{d}z = \int_A (\vec{\nabla} \times \vec{F}^*)_z \mathrm{d}A + \mathrm{i} \int_A \vec{\nabla} \cdot \vec{F}^* \mathrm{d}A$$
$$= 0 + \mathrm{i} \int_A \vec{\nabla} \cdot \vec{F}^* \mathrm{d}A = 2\pi\mathrm{i} \int_A \delta^{(2)}(x,y)\, \mathrm{d}A = 2\pi\mathrm{i}\,. \tag{1.131}$$

We have derived a connection of the Cauchy residue theorem with the divergence theorem, and Stokes's theorem.

Chapter 2

Cauchy's Residue Theorem and Branch Cuts

2.1 Taylor and Laurent Series

2.1.1 Taylor Series

You have probably heard about Taylor expansions, which for a function $f = f(x)$ about the origin can be written as

$$f(x) = f(0) + f'(0)\,x + \frac{1}{2!}f''(0)\,x^2 + \cdots = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}\,x^n = \sum_{n=0}^{\infty} a_n\,x^n\,. \tag{2.1}$$

Here, the a_n with $n = 0, 1, 2, \ldots$ are constant coefficients. In the complex domain, one has

$$f(z) = f(0) + f'(0)\,z + \frac{1}{2!}f''(0)\,z^2 + \cdots = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}\,z^n = \sum_{n=0}^{\infty} a_n\,z^n\,. \tag{2.2}$$

One hopes that the series in z converges. This is manifest in the condition

$$\left| f(z) - \sum_{n=0}^{M} \frac{f^{(n)}(0)}{n!}\,z^n \right| \leq C\,|z|^{M+1}\,, \qquad |z| < R\,. \tag{2.3}$$

Here, $C > 0$ is a constant. If such a condition holds, we say that

$$f(z) = \sum_{n=0}^{M} \frac{f^{(n)}(0)}{n!}\,z^n + \mathcal{O}(z^{M+1}) \tag{2.4}$$

In the lecture, we will generalize to a point other than the origin.

2.1.2 Laurent Series

However, functions like

$$g(z) = \frac{1}{z^4 \sin(z)} \tag{2.5}$$

obviously cannot be expanded in a Taylor series about $z = 0$. At best, we can do the following expansion,

$$\sin(z) = z - \frac{z^3}{3!} + \frac{z^5}{5!} + \dots \,, \tag{2.6}$$

and so

$$\begin{aligned} g(z) = \frac{1}{z^4 \sin(z)} &= \frac{1}{z^4 \left(z - \dfrac{z^3}{3!} + \dfrac{z^5}{5!} + \dots \right)} = \frac{1}{z^5 \left(1 - \dfrac{z^2}{3!} + \dfrac{z^4}{5!} + \dots \right)} \\ &= \frac{1}{z^5} + \frac{1}{6\, z^3} + \frac{7}{360\, z} + \frac{31\, z}{15120} + \mathcal{O}(z^3) \,. \end{aligned} \tag{2.7}$$

This expansion obviously does not start from the term of order zero, but from a term proportional to z^{-5}. It is called a Laurent expansion. The general formula reads

$$g(z) = \sum_{n=-\infty}^{\infty} a_n \, z^n \,. \tag{2.8}$$

It starts at $n = -\infty$ instead of $n = 0$, in contrast to the Taylor expansion. Of course, we can formulate a Laurent expansion about a point z_0, which reads

$$g(z) = \sum_{n=-\infty}^{\infty} b_n \, (z - z_0)^n \,, \tag{2.9}$$

with different coefficients b_n, but let us stick for the moment with the expansion (2.8). (If all coefficient b_n with $n < 0$ vanish, we say that $g(z)$ is analytic about the point $z = z_0$. If all a_n's with $n < -M$ will vanish, then we say that g has an Mth order pole at the origin.)

2.1.3 Toward Cauchy

Of preeminent importance is the integral

$$I = \oint g(z) \, \mathrm{d}z = \int_C g(z) \, \mathrm{d}z = \int_C \left(\sum_{n=-\infty}^{\infty} a_n \, z^n \right) \mathrm{d}z \,, \tag{2.10}$$

where the contour C is an anticlockwise circle (taken in the mathematically positive sense) of radius R around the origin. We shall see that only a very limited number of a_n coeffcients (in fact, just one of them) contributes to the integral. Let us therefore consider the integral

$$J = \oint_C \frac{1}{z^m} \, \mathrm{d}z \,, \qquad z = R \, \exp(\mathrm{i}\theta) \,, \qquad \theta \in (0, 2\pi) \,, \tag{2.11}$$

where $z = z(\theta)$ thus describes an anticlockwise circle about the origin. Furthermore, m will be assumed to be an integer. Now, for $m \neq 1$, we have

$$J = \int_0^{2\pi} \mathrm{d}\theta \; (\mathrm{i}R) \, \exp(\mathrm{i}\theta) \, [R \exp(\mathrm{i}\theta)]^{-m} = \mathrm{i}R^{1-m} \int_0^{2\pi} \mathrm{d}\theta \, \exp[-\mathrm{i}(m-1)\theta] \tag{2.12}$$

$$= \mathrm{i}R^{1-m} \left[\frac{1}{-(m-1)\mathrm{i}} \, \exp[-\mathrm{i}(m-1)\theta] \right]_{\theta=0}^{\theta=2\pi} = -R^{1-m} \left[\frac{1}{(m-1)} \, \exp[-\mathrm{i}(m-1)\theta] \right]_{\theta=0}^{\theta=2\pi} = 0 \,, \quad m \neq 1 \,.$$

The easiest way to treat the case $m = -1$ is by an explicit calculation, just for this case. However, for $m = 1$, we can alternatively replace $m - 1 \to \epsilon$ and do a Taylor expansion for small ϵ. In this calculation, the replica trick becomes useful, in the form

$$R^{-\epsilon} = \exp[-\epsilon \, \ln(R)] = 1 - \epsilon \, \ln(R) + \mathcal{O}(\epsilon^2) \, . \tag{2.13}$$

One obtains

$$\begin{aligned} \lim_{m \to 1} J = & \, - R^{-\epsilon} \, \left[\frac{1}{\epsilon} \, \exp(-\mathrm{i} \epsilon \theta) \right]_{\theta=0}^{\theta=2\pi} = - \lim_{\epsilon \to 0} \left[\frac{1}{\epsilon} \, (1 - \epsilon \, \ln(R)) \, (1 - \mathrm{i} \epsilon \theta) \right]_{\theta=0}^{\theta=2\pi} \\ = & \, \left[-\frac{1}{\epsilon} + \ln(R) + \mathrm{i} \, \theta \right]_{\theta=0}^{\theta=2\pi} = [\mathrm{i} \, \theta]_{\theta=0}^{\theta=2\pi} = 2\pi \, \mathrm{i} \, . \end{aligned} \tag{2.14}$$

We note that the term $\ln(R)$ is independent of θ. Of course, this result could have been obtained by a direct calculation, without letting $m \to 1$, but the above derivation illustrates that the special case $m = 1$ actually follows from the more general case by a limiting process. For a function $g(z)$ that has the Laurent expansion $g(z) = \sum_{n=-\infty}^{\infty} a_n \, z^n$, we therefore have

$$I = \oint_C \mathrm{d}z \, f(z) = \oint_C \mathrm{d}z \, \left(\sum_{m=-\infty}^{\infty} a_m \, z^m \right) = 2\pi \, \mathrm{i} \, a_{-1} \equiv 2\pi \, \mathrm{i} \, \left(\operatorname*{Res}_{z=0} \, f(z) \right) \, , \tag{2.15}$$

where the last term constitutes a definition of the residue

$$\operatorname*{Res}_{z=0} \, f(z) \equiv a_{-1} \, . \tag{2.16}$$

Only the coefficient a_{-1} contributes. We write this as

$$\oint_C \mathrm{d}z \, f(z) = 2\pi \, \mathrm{i} \, \operatorname*{Res}_{z=0} \, f(z) \, . \tag{2.17}$$

Since closed contours in the complex z plane do not normally contribute any nonvanishing value to an integral, this result can be generalized easily. We have for an expansion about z_0, the Laurent expansion

$$f(z) = \sum_{m=-\infty}^{\infty} b_m \, (z - z_0)^m \, . \tag{2.18}$$

A contour integral that encircles z_0 in the mathematically positive sense, can be written as

$$\oint_{C_0} \mathrm{d}z \, f(z) = 2\pi \, \mathrm{i} \, b_{-1} = 2\pi \, \mathrm{i} \, \operatorname*{Res}_{z=z_0} \, f(z) \, . \tag{2.19}$$

Closed contour integrals in regions where the integrand is analytic, simply vanish. This enables us to generalize the result as follows. For a contour C that encircles n residues located at point $z = z_i$ with $i \in \{1, \ldots, n\}$,

$$\oint_C \mathrm{d}z \, f(z) = 2\pi \, \mathrm{i} \, \sum_{i=1}^{n} \operatorname*{Res}_{z=z_i} \, f(z) \, . \tag{2.20}$$

This is Cauchy's residue theorem.

2.1.4 Single Poles and Higher Orders

For functions that have a single pole, like

$$g(z) = \frac{1}{\sin z} \approx \frac{1}{z - \frac{1}{3} \, z^3 + \ldots} \, , \qquad \operatorname*{Res}_{z=0} \, g(z) = 1 \, , \tag{2.21}$$

the calculation of the residue is obvious. For functions that have poles of higher order, it becomes more complicated. We have already derived that

$$\operatorname*{Res}_{z=0}\left(\frac{1}{z^4\sin(z)}\right)=\frac{7}{360}\,. \tag{2.22}$$

Let us also consider

$$g(z)=\frac{\cos(z)}{z^4\sin(z)}=\frac{1}{z^5}\frac{z\cos(z)}{\sin(z)}\,. \tag{2.23}$$

Now, a simple Taylor expansion of numerator and denominator shows that

$$\frac{z\cos(z)}{\sin(z)}=1-\frac{z^2}{3}-\frac{z^4}{45}+\dots \tag{2.24}$$

and so, for $z\to 0$,

$$g(z)\approx\frac{1}{z^5}\left(1-\frac{z^2}{3}-\frac{z^4}{45}+\dots\right),\qquad\qquad \operatorname*{Res}_{z=0}\,g(z)=-\frac{1}{45}\,. \tag{2.25}$$

Another example is

$$\frac{1}{4!}\,\frac{\mathrm{d}^4}{\mathrm{d}z^4}\left\{z^5\,\left(\frac{\cos(z)}{z^4\sin(z)}\right)\right\}\Bigg|_{z=0}=-\frac{1}{45}\,. \tag{2.26}$$

2.1.5 Useful Generalization

Let us now investigate a generalization of this result, namely, the case where $f(z)$ has an Mth order pole. For the example in Eq. (2.25), we have $M=5$. We are interested in finding out about the term of order $(z-z_0)^{-1}$ in $f(z)$. To this end, one can follow the *ad hoc* procedure outlined above: We just expand numerator and denominator to the required order and then read off the term of order $(z-z_0)^{-1}$. However, it is also possible to follow a more systematic approach. If one multiplies the terms $\{a_{-M}\,(z-z_0)^{-M},a_{-M+1}\,(z-z_0)^{-M+1},\dots,a_{-1}\,(z-z_0)^{-1},\dots\}$ by a factor $(z-z_0)^M$, then they transform into the set $\{a_{-M},a_{-M+1}\,(z-z_0),\dots,a_{-1}\,(z-z_0)^{M-1},\dots\}$. Expressed differently,

$$f(z)=\frac{a_{-M}}{(z-z_0)^M}+\frac{a_{-M+1}}{(z-z_0)^{M-1}}+\dots\frac{a_{-1}}{(z-z_0)}+\dots+a_n\,(z-z_0)^n+\dots\,, \tag{2.27}$$

$$(z-z_0)^M\,f(z)=a_{-M}+(z-z_0)\,a_{-M+1}+\dots+(z-z_0)^{M-1}\,a_{-1}+\dots\,. \tag{2.28}$$

If we differentiate the expression $(z-z_0)^M\,f(z)$ a total of $M-1$ times with respect to z, and set $z=z_0$ after the differentiation, then the only contributing term is the one proportional to a_{-1}. Terms of lower order are explicitly annihilated by the differential operator, and terms of higher order give rise to positive powers of $(z-z_0)$; these are annihilated if we set $z=z_0$ after the differentiation. This leads to the general formula, valid for an Mth order pole,

$$\operatorname*{Res}_{z=z_0}\,f(z)=\frac{1}{(M-1)!}\left[\frac{\mathrm{d}^{M-1}\left\{(z-z_0)^M\;f\,(z)\right\}}{\mathrm{d}z^{M-1}}\right]_{z=z_0}\,. \tag{2.29}$$

Other examples are given by the relations,

$$\operatorname*{Res}_{z=0}\left(\frac{1}{z^4}\exp(z)\right)=\frac{1}{6}\,,\qquad\operatorname*{Res}_{z=0}\left(\frac{1}{z^5}\exp(z)\right)=\frac{1}{24}\,,\qquad\operatorname*{Res}_{z=0}\left(\frac{1}{z^5}\frac{\exp(\mathrm{i}z)}{\sin(z)}\right)=0\,. \tag{2.30}$$

Ad hoc exercise: Show that

$$\operatorname*{Res}_{z=0} \frac{1}{z(z-1)} = -1\,, \qquad \operatorname*{Res}_{z=1} \frac{1}{z(z-1)} = 1\,. \tag{2.31}$$

Be careful in reading precisely the written mathematical expressions.

2.1.6 Cauchy Theorem and Integrals

Let us consider a specific integral,

$$I = \int_{-\infty}^{\infty} \mathrm{d}x\, \frac{1}{x^2+4}\,. \tag{2.32}$$

This integral is, first and foremost, an integral along the real axis, which can be promoted to a complex contour integral,

$$I = \int_{-\infty}^{\infty} \mathrm{d}t\, \frac{1}{t^2+4}\,. = \int_{-\infty}^{\infty} \mathrm{d}t\, \frac{\mathrm{d}z(t)}{\mathrm{d}t}\, \frac{1}{[z(t)]^2+4} = \int\limits_{C(-\infty,\infty)} \mathrm{d}z\, \frac{1}{z^2+4}\,. \tag{2.33}$$

Here, $C(-\infty,\infty)$ is a complex integration integration contour, which starts at $z_1 = -\infty$ and goes along the entire real axis, to end at $z_2 = +\infty$. A suitable parameterization, in the sense of our considerations outlined above, is $z(t) = t = t + \mathrm{i}\,0$.

A question now is whether or not we can close the contour along a half-circle of radius $R \to \infty$, in the upper half of the complex plane. The addition of the contribution of the half circle can be described by the replacement

$$C(-\infty,\infty) \to C(-\infty,\infty) + C_{\rm up}(R\to\infty) \tag{2.34}$$

where $C_{\rm up}(R\to\infty)$ is the contour parameterized as

$$z(\theta) = R\,\exp(\mathrm{i}\theta)\,, \qquad 0 < \theta < \pi\,, \qquad R\to\infty\,. \tag{2.35}$$

The limit $R\to\infty$ is to be taken at the end of the calculation.

We can use the following argument. Suppose that we fly, in a small private propeller-driven aircraft, from the Rolla/Vichy airport, to Memphis. The work integral is

$$W = \int \vec{F}\cdot \mathrm{d}r \le |\vec{F}_{\rm max}|\,|\Delta\vec{\ell}|\,, \tag{2.36}$$

where $|\vec{F}_{\rm max}|$ is the maximum force exerted by the propeller during any phase of the flight (probably during lift-off), and $|\Delta\vec{\ell}|$ is the total distance traveled. Likewise, for any complex contour integral, we have the inequality

$$\left| \int f(z)\,\mathrm{d}z \right| \le |f(z)|_{\rm max}\,\mathcal{L}\,, \tag{2.37}$$

where $|f(z)|_{\rm max}$ is the maximum modulus of the integrand along the contour, and $\mathcal{L}$ is the length of the contour. Also, for $R\to\infty$, one has

$$|z^2+4| = \left|R^2\,\exp(2\mathrm{i}\theta)+4\right| \approx \left|R^2\,\exp(2\mathrm{i}\theta)\right| = R^2\,. \tag{2.38}$$

For the half-circle at $R\to\infty$, we thus have

$$\left| \int\limits_{C_{\rm up}(R\to\infty)} \mathrm{d}z\, \frac{1}{z^2+4} \right| \le \frac{1}{R^2}\,(\pi R) = \frac{\pi}{R} \to 0\,, \qquad R\to\infty\,. \tag{2.39}$$

We can thus write

$$I = \int\limits_{C(-\infty,\infty)+C_{\rm up}(R\to\infty)} {\rm d}z\, \frac{1}{z^2+4} = 2\pi{\rm i}\, \operatorname*{Res}_{z=2{\rm i}} \frac{1}{z^2+4}\,. \tag{2.40}$$

We have used, here, the fact that the only poles of the function

$$f(z) = \frac{1}{z^2+4}\,. \tag{2.41}$$

are at $z = 2{\rm i}$ and at $z = -2{\rm i}$. In fact, a partial fraction decomposition with the *ansatz*

$$f(z) = \frac{A}{z+2{\rm i}} + \frac{B}{z-2{\rm i}} \tag{2.42}$$

yields

$$\begin{aligned} f(z) &= \frac{A(z-2{\rm i})}{z^2+4} + \frac{B(z+2{\rm i})}{z^2+4} \\ &= \frac{(A+B)z - 2{\rm i}\,(A-B)}{z^2+4}\,. \end{aligned} \tag{2.43}$$

The resulting system of equations has the solution

$$A+B = 0\,, \qquad A-B = -\frac{1}{2{\rm i}} \quad \Rightarrow \quad A = -B = -\frac{1}{4{\rm i}}\,. \tag{2.44}$$

Hence,

$$f(z) = \frac{1}{z^2+4} = -\frac{1}{4{\rm i}}\,\frac{1}{z+2{\rm i}} + \frac{1}{4{\rm i}}\,\frac{1}{z-2{\rm i}}\,. \tag{2.45}$$

This representation has the form of a sum over coefficients, multiplying singular terms of the form $1/(z-z_0)$. From this representation, we can immediately read off that

$$\operatorname*{Res}_{z=2{\rm i}} \frac{1}{z^2+4} = \frac{1}{4{\rm i}}\,, \qquad \operatorname*{Res}_{z=-2{\rm i}} \frac{1}{z^2+4} = -\frac{1}{4{\rm i}}\,. \tag{2.46}$$

Finally, we can complete the calculation outlined in Eq. (2.40),

$$I = \int\limits_{C(-\infty,\infty)+C_{\rm up}(R\to\infty)} {\rm d}z\, \frac{1}{z^2+4} = 2\pi{\rm i} \operatorname*{Res}_{z=2{\rm i}} \frac{1}{z^2+4} = 2\pi{\rm i}\frac{1}{4{\rm i}} = \frac{\pi}{2}\,. \tag{2.47}$$

It somehow quite miraculous that one can verify the integral (2.32) on the basis of a complex generalization of the integral, by adding the (vanishing) contribution of a half circle in the upper half of the complex plane, and then, reducing the integral to the evaluation of the integrand in a small region around a single point.

Likewise, if we close the contour in the lower half of the complex plane, we end up with a replacement analogous to Eq. (2.34),

$$C(-\infty,\infty) \to C(-\infty,\infty) + C_{\rm down}(R\to\infty)\,, \tag{2.48}$$

where $C_{\rm down}(R\to\infty)$ is the contour parameterized as

$$z(\theta) = R\,\exp(-{\rm i}\theta)\,, \qquad 0 < \theta < \pi\,, \qquad R\to\infty\,. \tag{2.49}$$

The reversal of the sense of revolution implies an additional minus sign, to yield

$$I = \int\limits_{C(-\infty,\infty)+C_{\rm down}(R\to\infty)} {\rm d}z\, \frac{1}{z^2+4} = (-2\pi{\rm i}) \operatorname*{Res}_{z=-2{\rm i}} \frac{1}{z^2+4} = (-2\pi{\rm i})\left(-\frac{1}{4{\rm i}}\right) = \frac{\pi}{2}\,. \tag{2.50}$$

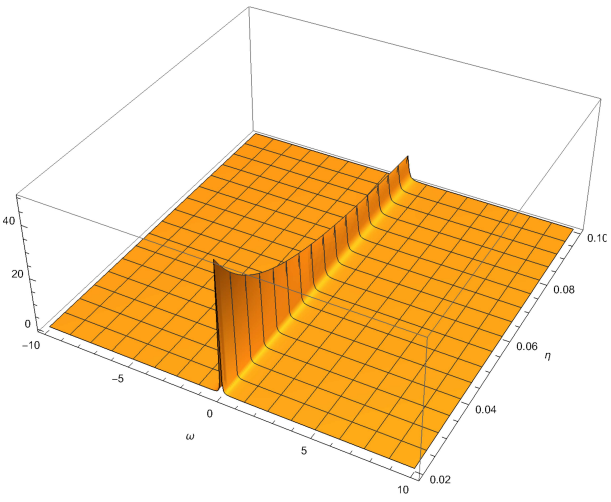

Figure 2.1: Convergence of the function $f_\eta(\omega)$ given in Eq. (2.53) toward a Dirac-δ function, for small η.

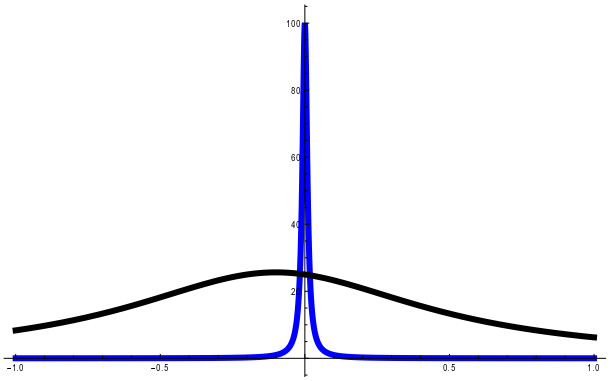

Figure 2.2: Illustration on Eqs. (2.62) and (2.67). The black curve is a sample function $g(\omega)$, while $f_\eta(\omega)$ is represented by the blue curve.

This confirms the result given in Eq. (2.40)

A numerical investigation of the integral given in Eq. (2.32)

$$I = \int_{-\infty}^{\infty} \mathrm{d}x \, \frac{1}{x^2+4} \, . \tag{2.51}$$

is left as an exercise to the reader. Observe that the convergence will be slow if we interpret the numerical limits of the integration domain as

$$I = \lim_{\Lambda\to\infty} \int_{-\Lambda}^{\Lambda} \mathrm{d}x \, \frac{1}{x^2+4} \, . \tag{2.52}$$

with the remainder term, as a function of Λ*, falling off only as* $1/\Lambda$*.*

2.2 Some Applications of Residue Calculus

2.2.1 Complex Contour Integrals and Delta Function

Yet another application, which has a connection to the Dirac-δ function, is as follows. Let us consider a function

$$f_\eta(\omega) = \frac{\eta}{\omega^2 + \eta^2}\,, \tag{2.53}$$

which resembles, for $\eta \to 0$, a Dirac–δ function [see also Fig. 2.1]. An integral such as

$$\int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\eta}{\omega^2 + \eta^2} = \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\eta}{(\omega + \mathrm{i}\,\eta)\,(\omega - \mathrm{i}\,\eta)}\,, \tag{2.54}$$

will be of prime importance, with the idea that η is small. We can close the integration contour either in the upper or the lower complex plane, because the half-circle integral behaves as $R^{-2}\,R \to 0$ for $R \to \infty$. At the singularity, at $\omega = \mathrm{i}\eta$, we have

$$\frac{\eta}{(\omega + \mathrm{i}\,\eta)\,(\omega - \mathrm{i}\,\eta)} \approx \frac{\eta}{2\,\mathrm{i}\,\eta\,(\omega - \mathrm{i}\,\eta)}\,, \tag{2.55}$$

and hence

$$\operatorname*{Res}_{\omega = \mathrm{i}\eta} \frac{\eta}{(\omega + \mathrm{i}\,\eta)\,(\omega - \mathrm{i}\,\eta)} = \frac{\eta}{2\,\mathrm{i}\,\eta} = \frac{1}{2\,\mathrm{i}}\,. \tag{2.56}$$

The result is

$$\int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\eta}{\omega^2 + \eta^2} = 2\pi\,\mathrm{i}\,\frac{1}{2\,\mathrm{i}} = \pi\,. \tag{2.57}$$

Reversing the argument, while closing the contour in the lower half of the complex plane, we have

$$\int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\eta}{\omega^2 + \eta^2} = (-2\pi\,\mathrm{i})\,\left(-\frac{1}{2\,\mathrm{i}}\right) = \pi\,. \tag{2.58}$$

The first minus sign is due to the reversed sense of revolution around the singularity, the second, because the sign of the residue at $\omega = -\mathrm{i}\eta$ changes sign.

Now, it is clear, from the graphical representation in Fig. (2.1), that the smaller η is, the smaller is the full width at half maximum of the function. We consider the following relations,

$$f_\eta(\omega) = \frac{\eta}{\omega^2 + \eta^2}\,, \qquad f_\eta(\eta) = \frac{1}{2\eta}\,, \qquad f_\eta(-\eta) = \frac{1}{2\eta}\,, \qquad f_\eta(0) = \frac{1}{\eta}\,. \tag{2.59}$$

It becomes evident that the value $f_\eta(\pm\eta)$ is half the value at the maximum, $f_\eta(0)$. The full width at half maximum (FHWM) is defined as the difference of the arguments of the function $f_\eta(\omega)$ where the function assumes half its maximum value:

$$\mathrm{FWHM} = \eta - (-\eta) = 2\eta\,. \tag{2.60}$$

As $\eta \to 0^+$, the FWHM goes to zero, while the maximum of the value of f_η at $\omega = 0$ goes to infinity,

$$\lim_{\eta\to 0}\lim_{\omega\to 0} f_\eta(\omega) = \lim_{\eta\to 0}\frac{1}{\eta} = \infty\,, \qquad \lim_{\omega\to 0}\lim_{\eta\to 0} f_\eta(\omega) = \lim_{\omega\to 0} 0 = 0\,. \tag{2.61}$$

This illustrates how careful one has to be with interchanging limiting processes.

Let us now consider the following functional,

$$\Delta[g] = \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega\, f_\eta(\omega)\, g(\omega)\,. \tag{2.62}$$

One puts in a test function g and gets a real number as a result. Let ℓ be a characteristic scale over which the function $g(\omega)$ varies significantly. Then, provided $\eta \ll \ell$, we can approximate

$$g(\omega) \approx g(0) \tag{2.63}$$

under the integral sign, in the evaluation of the functional $\Delta[g]$. For $|\omega| \gg \eta$, the integrand function

$$f_\eta(\omega)\, g(\omega) \to 0\,, \qquad |\omega| \gg \eta\,, \qquad \eta \to 0^+\,, \tag{2.64}$$

because the function $f_\eta(\omega)$ tends to zero there. Hence, we can write [see also Fig. 2.2]

$$\Delta[g] = \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega\, f_\eta(\omega)\, g(\omega) = g(0) \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega\, f_\eta(\omega) = \pi\, g(0)\,. \tag{2.65}$$

Furthermore, let $a < 0$ and $b > 0$ be (finite) real numbers, and let us investigate the integral

$$\Delta_{ab}[g] = \lim_{\eta\to 0^+} \int_a^b \mathrm{d}\omega\, f_\eta(\omega)\, g(\omega)\,. \tag{2.66}$$

In this case, one can show that the integration intervals $\omega \in (-\infty, a)$ and $\omega \in (b, \infty)$ yield a vanishing contribution to the integrals, because the integrand can only be of order η in both intervals. Hence, we can establish that [see also Fig. 2.2]

$$\Delta_{ab}[g] = \lim_{\eta\to 0^+} \int_a^b \mathrm{d}\omega\, f_\eta(\omega)\, g(\omega) = \pi\, g(0)\,, \qquad \lim_{\eta\to 0^+} \int_a^b \mathrm{d}\omega\, f_\eta(\omega) = \pi\,, \tag{2.67}$$

These equations bear a striking similarity to the defining equations of the Dirac-δ function,

$$\Delta_{ab}[g] = \int_a^b \mathrm{d}\omega\, \delta(\omega)\, g(\omega) = g(0)\,, \qquad \int_a^b \mathrm{d}\omega\, \delta(\omega) = 1\,, \tag{2.68}$$

except that, in the latter equations, the multiplicative factor π is missing.

We can establish that $f_\eta(\omega)$ is a valid representation of π times the Dirac-δ function, if we use $f_\eta(\omega)$ under an integral sign, and take the limit $\eta \to 0^+$ after the integrals have been evaluated. With the proviso that the limit $\eta \to 0^+$ be taken after the integrals have been evaluated (a necessity indicated by the dot over the equal sign in the equation below), we can establish that

$$\delta(\omega) \doteq \lim_{\eta\to 0^+} \frac{\eta}{\pi(\omega^2 + \eta^2)}\,, \tag{2.69}$$

Or, in the sense of a distribution, one has

$$f_\eta(\omega) = \frac{\eta}{\omega^2 + \eta^2} \doteq \pi\delta(\omega)\,, \qquad \eta \to 0^+\,. \tag{2.70}$$

2.2.2 Mittag–Leffler (Pole) Expansions

We start by considering functions of the form

$$f(z) = \frac{g(z)}{g'(z)}\,, \tag{2.71}$$

and analyze their behavior near a zero of the function $g(z)$. If we have

$$g(z) = g(z_0) + g'(z_0)\,(z - z_0) + \frac{1}{2!}\, g''(z_0)\,(z - z_0)^2 + \dots\,, \qquad g(z_0) = 0\,, \tag{2.72}$$

in the vicinity of $z = z_0$, then we should replace, for the sake of the calculation of the residue at $z = z_0$,

$$g'(z) \to g'(z_0)\,(z - z_0)\,, \tag{2.73}$$

resulting in the relation

$$f(z) = \frac{g'(z_0)}{g'(z_0)\,(z - z_0)} + \text{const.} = \frac{1}{(z - z_0)} + \text{const.}\,, \tag{2.74}$$

demonstrating the property that $f(z)$ has unit residue at $z = z_0$.

A prime example of a function which has the structure (2.71) is the example

$$f(z) = \cot(z) = \frac{\cos(z)}{\sin(z)}\,, \qquad \frac{\mathrm{d}}{\mathrm{d}z}\sin(z) = \cos(z)\,. \tag{2.75}$$

Singularities of the complex cotangent are exactly at those places where the function $\sin(z)$ has zeros. On the other hand, we have

$$\sin(z) = 0\,, \qquad z = n\pi\,, \qquad n \in \mathbb{Z}\,. \tag{2.76}$$

This property illustrates that $f(z) = \cot(z)$ has unit residue at $z = n\pi$, and otherwise constitutes a *meromorphic function* in the complex plane.

Let us try to reconstruct $\cot(z)$ from its behavior near the sigularities. This will be called a Mittag–Leffler (pole) expansion. In fact, we can say that the decomposition (2.45) is a special, and conceptually very simple, case of a so-called Mittag–Leffler expansion, which is based on the idea that the singularities of a complex function carry a lot of global information on the function over the entire complex plane. Indeed, from the position of the singularities and the corresponding residues, one may derive global properties of a complex function, such as the value of any closed-contour integral in the complex plane. Mittag–Leffler expansions take this idea a step further and attempt to represent functions as sums over their pole terms.

The Mittag–Leffler theorem itself makes only a very cursory and not very helpful statement in this regard. Roughly, it reads as follows. Let D be an open set in $\mathbb{C}$ and $E \subset D$ a closed discrete subset. For each a in E, let $p_a(z)$ be a polynomial in $1/(z - a)$. There is a meromorphic function f on D such that for each $a \in E$, the function $f(z) - p_a(z)$ has only a removable singularity at a *(i.e., the difference of $f(z)$ and $p_a(z)$ is well-behaved, possibly even zero).* In particular, the principal part of f at a is $p_a(z)$. End of Theorem.

So, in some sense, we can say that the Mittag–Leffler theorem says that, given a polynomial in inverse powers of $z - a$, we can find a meromorphic function $f(z)$ which approximates the given polynomial in inverse powers of $z - a$ quite well, within a certain region of the complex plane.

This is in principle very nice, but we would like more. We would like equality. Let us therefore investigate whether or not we can say that

$$\begin{aligned} f(z) = \cot(z) &= \frac{\cos(z)}{\sin(z)} \\ &\stackrel{!?}{=} \sum_{n\in\mathbb{Z}} \frac{1}{z - n\pi} = \frac{1}{z} + \sum_{k=1}^{\infty}\left(\frac{1}{z - k\pi} + \frac{1}{z + k\pi}\right) = \frac{1}{z} + \sum_{k=1}^{\infty}\frac{2z}{z^2 - (k\pi)^2}\,. \end{aligned} \tag{2.77}$$

Let us do a numerical experiment. A calculation reveals that, for the reference value $z = z_R = 0.09$, we have

$$\cot(z_R) = 11.081095\,. \tag{2.78}$$

If we compare this with the partial sums of the series in Eqs. (2.77), we find

$$f(z, K_{\max}) = \frac{1}{z_R} + \sum_{k=1}^{K_{\max}} \frac{2z}{z^2 - (k\pi)^2}\,, \tag{2.79}$$

$$f(z = z_R, K_{\max} = 5) = 11.084402\,, \tag{2.80}$$

$$f(z = z_R, K_{\max} = 100) = 11.081276\,, \tag{2.81}$$

$$f(z = z_R, K_{\max} = 10000) = 11.081096\,, \tag{2.82}$$

$$f(z = z_R, K_{\max} = 100000) = 11.081095 \approx \cot(z_R)\,. \tag{2.83}$$

The last given approximate equality already holds up to eight decimals.

In fact, one can show in a mathematically rigorous way, based on additional considerations beyond our scope here, that the conjectured relation (2.77) indeed holds, so that

$$\cot(z) = \frac{1}{z} + \sum_{k=1}^{\infty} \frac{2z}{z^2 - (k\pi)^2}\,, \qquad z \neq n\pi\,, \qquad n \in \mathbb{Z}\,. \tag{2.84}$$

The sum converges for any $z \in \mathbb{C}$. *Proof: Exercise.*

Another unmarked exercise: In view of the sign-alternating behavior of the sine function, we can ascertain that

$$\operatorname*{Res}_{z=n\pi} \frac{1}{\sin(z)} = (-1)^n\,. \tag{2.85}$$

An almost trivial generalization of the considerations above leads to the relation

$$\frac{1}{\sin(z)} = \sum_{n\in\mathbb{Z}} \frac{(-1)^n}{z - n\pi} = \frac{1}{z} + \sum_{k=1}^{\infty} \frac{2\,(-1)^k\, z}{z^2 - (k\pi)^2}\,, \qquad z \neq n\pi\,, \qquad n \in \mathbb{Z}\,. \tag{2.86}$$

This function carries the special name of a cosecans, $\csc(z) = 1/\sin(z)$.

In many cases, one can reconstruct a function from its behavior near singularities, leading to a very economical representation, and quite marvelous, and useful, series representations of special functions.

2.3 Branch Cuts and Dispersion Relations

2.3.1 Connection to the "International Date Line"

Let us go on a detour and consider the time zones on the Earth. If it is noon here, then it is 1PM in New York City, 7PM in Paris, France, 10PM in Dubai, and the more we head eastwards on the planet, the later it gets. In Sydney, Australia, it will be 5AM on the next day. Conversely, if it is noon here, then it is 10AM in Los Angeles, and in Hawaii, it is just 8AM in the morning. This is strange. Somehow, it cannot be that the more we head eastwards, the later it gets, and the more we head westwards, the earlier it gets. There must be a "branch cut" somewhere, i.e., an international date line, where the day jumps. By international convention, it occurs in the middle of the Pacific Ocean, exactly on the opposite side of the Earth as compared to Greenwich, London, UK, which defines the universal time zone (UTC).

Some idiosyncracies exist: Papeete in French Polynesia is in the time zone UTC-11, while the central Pacific Repulic of Kiribati is in UTC+14, even though it is east of Papeete. These indiosyncracies have historic and

cultural reasons. The important point for us is that the existence of the "branch cut" (the international date line) is necessary.

As one cross the international date line westwards, one "loses a day". When Magellan traveled the world, westwards, from 1519 to 1522, he did not know about the international date line. When one crosses the international date line westwards, one has to switch the date one day into the future, in order to keep consistency with everyone else. However, Magellan's seamen did not know that they "lost a day", and, according to their own time keeping, arrived one day earlier than they started. Upon return, they celebrated Holy Mass on a Saturday as opposed to a Sunday. That is how they could tell that they really surrounded the World. The Straight of Magellan in South America stills bears testimony to their exploits.

After this detour, let us explore if a similar phenomenon exists in regard to the square root function in the complex plane. One can represent a complex number in two ways, either by considering the real and imaginary parts, or, by considering its modulus and its complex argument,

$$z = x + \mathrm{i}\, y\,, \qquad z = |z|\, \exp(\mathrm{i}\varphi)\,, \qquad \varphi = \arg(z)\,. \tag{2.87}$$

Here, φ is the complex argument (complex phase) of the complex number z. First, a word of caution. One often writes the equation

$$\varphi = \arctan(y/x)\,. \tag{2.88}$$

However, this equation should be taken with a grain of salt.

We may illustrate the problems by way of example. Let us take two complex numbers $z = z_1$ and $z = z_2$, as follows,

$$z = z_1 = \sqrt{2} + \mathrm{i}\,\sqrt{2}\,, \qquad x_1 = y_1 = \sqrt{2}\,, \qquad z = z_2 = -\sqrt{2} - \mathrm{i}\,\sqrt{2}, \qquad x_2 = y_2 = -\sqrt{2}\,. \tag{2.89}$$

In both cases, one has the complex modulus

$$|z_1| = |z_2| = \sqrt{2^2 + 2^2} = \sqrt{4} = 2\,. \tag{2.90}$$

The complex phase, at face value, is

$$\varphi_1 = \arctan\left(\frac{\sqrt{2}}{\sqrt{2}}\right) = \varphi_2 = \arctan\left(\frac{(-\sqrt{2})}{(-\sqrt{2})}\right) = \frac{\pi}{4}\,. \tag{2.91}$$

However, this cannot be taken seriously because z_1 and z_2 are manifestly different complex numbers (with the same complex modulus $\sqrt{2}$, though). In fact, we have $z_1 + z_2 = 0$. The definition (2.88) is applicable only for $x > 0$, i.e., in the first and fourth quadrants of the complex plane. In the following, we shall use the assumption that

$$-\pi < \varphi \leq \pi\,, \tag{2.92}$$

i.e., that the range of the complex phase is chosen so that the entire complex plane can be covered. For a complex number which happens to be equal to a positive real number, we choose φ to be equal to zero. For a complex number in the upper half of the complex plane, we have $0 < \varphi < \pi$. For a complex number in the lower half of the complex plane, we have $-\pi < \varphi < 0$.

Hence, we write

$$\varphi = \arg z = \arctan\left(\frac{y}{x}\right) + \begin{cases} \pi & z = |z|\, \exp\left[\mathrm{i}(\arctan\left(\frac{y}{x}\right) + \pi)\right] \;\wedge\; -\pi < \arctan\left(\frac{y}{x}\right) + \pi \leq \pi \\ 0 & z = |z|\, \exp\left[\mathrm{i}\arctan\left(\frac{y}{x}\right)\right] \;\wedge\; -\pi < \arctan\left(\frac{y}{x}\right) \leq \pi \\ -\pi & z = |z|\, \exp\left[\mathrm{i}(\arctan\left(\frac{y}{x}\right) - \pi)\right] \;\wedge\; -\pi < \arctan\left(\frac{y}{x}\right) - \pi \leq \pi \end{cases} \tag{2.93}$$

Basically, this means: If you want to find $\varphi = \arg z$, then calculate the quantity $\arctan(y/x)$ and leave this result, or add or subtract π, so that the resulting φ reproduces $z = |z| \, \exp(\mathrm{i}\,\varphi)$, and so that $-\pi < \varphi \leq \pi$.

In our case, for $z = z_2$, we have

$$\varphi_2 = \arg z_2 = \frac{\pi}{4} - \pi = -\frac{3\pi}{4} \,. \tag{2.94}$$

This is alright beause z_2 is in the third quadrant of the complex plane.

Remark: One might think that a more accurate definition could be taken as

$$\varphi = -\mathrm{i} \ln \left(\frac{x + \mathrm{i}y}{\sqrt{x^2 + y^2}} \right) . \tag{2.95}$$

However, this definition is, in some sense, redundant. Namely, if we identify

$$z = x + \mathrm{i}y = |z| \, \exp(\mathrm{i}\varphi) \,, \qquad |z| = \sqrt{x^2 + y^2} \,, \tag{2.96}$$

then Eq. (2.95) *becomes somewhat redundant,*

$$\varphi = -\mathrm{i} \ln \left(\frac{|z| \, \exp(\mathrm{i}\varphi)}{|z|} \right) = -\mathrm{i} \, (\mathrm{i}\varphi) = \varphi \,. \tag{2.97}$$

Furthermore, the definition (2.95) *is actually valid only on the* principle branch *of the complex logarithm, as we shall see in the following. Still, it constitutes a useful specification of the cursory definition* (2.88)*.*

Note that, as far as the complex phase is concerned, in view of our conventions, the negative real axis constitutes an "international date line" as far as the complex phase of complex numbers is concerned.

Let us again consider two examples, namely, the complex argument of two complex numbers infinitesimally displaced from the negative real axis. One has, for a complex number $-4 + \mathrm{i}\,\epsilon$, which is infinitesimally above the negative real axis,

$$\lim_{\epsilon \to 0^+} \arg \left(-4 + \mathrm{i}\,\epsilon \right) = \pi \,, \qquad -4 = 4 \, \exp(\mathrm{i}\pi) \,. \tag{2.98}$$

For a complex number $-4 - \mathrm{i}\,\epsilon$, which is infinitesimally below the negative real axis, one has

$$\lim_{\epsilon \to 0^+} \arg \left(-4 - \mathrm{i}\,\epsilon \right) = \pi \,, \qquad -4 = 4 \, \exp(-\mathrm{i}\pi) \,. \tag{2.99}$$

The negative real axis acts as the "international date line" as far as the complex argument is concerned: infinitesimally above the negative real axis, the complex argument is $\varphi = \pi$, while infinitesimally below the negative real the complex argument is $\varphi = -\pi$. This does not matter too much because

$$\exp(\mathrm{i}\pi) = \exp(-\mathrm{i}\pi) = 1 \,, \tag{2.100}$$

but it has further consequences as we consider the complex square root function.

2.3.2 Branch Cut and Complex Square Root

If we consider the square root function, problems become apparent. We write the complex number z as

$$z = |z| \, \exp(\mathrm{i} \, \arg(z)) = |z| \, \exp(\mathrm{i}\,\varphi) \,, \qquad -\pi < \varphi \leq \pi \,. \tag{2.101}$$

We calculate the square root as follows,

$$\sqrt{z} = \sqrt{|z|} \, \exp(\mathrm{i} \, \arg(z)/2) = \sqrt{|z|} \, \exp(\mathrm{i}\,\varphi/2) \,, \qquad -\pi/2 < \varphi/2 \leq \pi/2 \,. \tag{2.102}$$

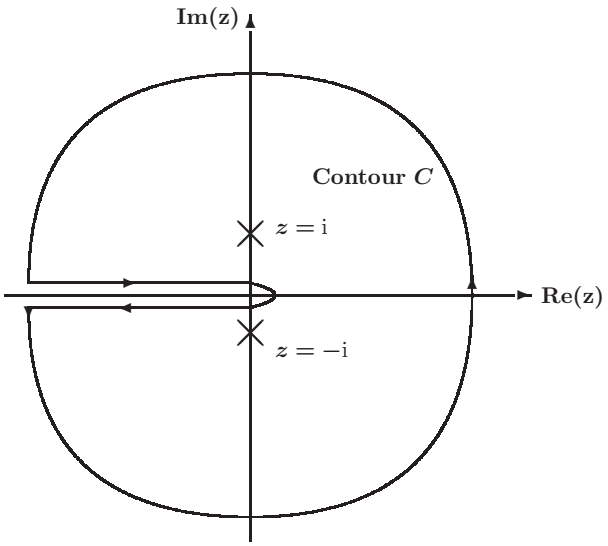

Figure 2.3: Contour C for the integral I given in Eq. (2.105).

From this formula, it becomes clear that the square root function has a discontinuity along the negative real axis,

By way of example, one has

$$\lim_{\epsilon \to 0^+} \sqrt{-4 + \mathrm{i}\,\epsilon} = 2\mathrm{i}\,, \tag{2.103}$$

while

$$\lim_{\epsilon \to 0^+} \sqrt{-4 - \mathrm{i}\,\epsilon} = -2\mathrm{i}\,. \tag{2.104}$$

The square root function changes sign along the negative real axis, it has a *branch cut* there.

In order to illustrate the use of the branch cut in a specific example, let us consider a specific complex contour integral, namely

$$I = \int_C \mathrm{d}z \frac{\sqrt{z}}{z^2 + 1}\,, \tag{2.105}$$

where C goes infinitesimally above the negative real axis from $-\infty$ to zero, and it goes infinitesimally below the real axis from 0 to $-\infty$ (see Fig. 2.3).

The modulus of the integrand, for large $|z|$, is proportional to $1/|z|^{3/2} \sim 1/R^{3/2}$. The length of the contour, at large radius, is proportional to $2\pi R$, where R is the radius of the circle. Therefore, the contribution of the (almost complete circle) to the integral vanishes. Therefore, with details being left to the reader to show, taking the difference of the integrand immediately above and below the branch cut, and observing that the integrand vanishes sufficiently fast at large radius in the one obtains

$$I = \int_C \mathrm{d}z \frac{\sqrt{z}}{z^2 + 1} = 2 \int_0^\infty \mathrm{d}x \frac{2\mathrm{i}\sqrt{x}}{x^2 + 1} = \sqrt{2}\pi\mathrm{i}\,. \tag{2.106}$$

An alternative way to evaluate the integral is as follows. One has

$$R_1 = \operatorname*{Res}_{z=\mathrm{i}} \frac{\sqrt{z}}{z^2 + 1} = -\frac{\mathrm{i}}{2} \exp\left(\frac{1}{4}\mathrm{i}\pi\right)\,, \tag{2.107}$$

while

$$R_2 = \operatorname*{Res}_{z=-\mathrm{i}} \frac{\sqrt{z}}{z^2+1} = \frac{\mathrm{i}}{2} \exp\left(-\frac{1}{4}\mathrm{i}\pi\right) . \tag{2.108}$$

The sum of the residues is, with details being left to the reader to show,

$$\begin{aligned} I &= 2\pi\mathrm{i}(R_1+R_2) = 2\pi\mathrm{i}\left[-\frac{\mathrm{i}}{2}\exp\left(\frac{1}{4}\mathrm{i}\pi\right) + \frac{\mathrm{i}}{2}\exp\left(-\frac{1}{4}\mathrm{i}\pi\right)\right] \\ &= 2\pi\mathrm{i}\left[\frac{1}{\sqrt{2}}\left(\frac{1}{2}-\frac{\mathrm{i}}{2}\right) + \frac{1}{\sqrt{2}}\left(\frac{1}{2}+\frac{\mathrm{i}}{2}\right)\right] = \frac{2\pi\mathrm{i}}{\sqrt{2}} = \sqrt{2}\pi\mathrm{i}\,. \end{aligned} \tag{2.109}$$

2.3.3 Ambiguity of the "International Date Line"

In the previous discussion, we have laid the branch cut of the complex square root function along the negative real axis. Colloquially speaking, we can say that, for about $99\,\%$ off all practical applications, this is all you need to know, and applying this concept will lead to the correct results.

However, a caveat should be mentioned. Namely, in theory, one could argue that the position of the international date line on the Earth could be redefined. Furthermore, if, say, the perceived center of civilization, at the point in time when the international date line was defined, had been, say, on the Midway Islands as opposed to Europe, then one might speculate that the definitions of UTC (universal time zone) and "international date line" would potentially have been reversed.

Conversely, there are some situations where one has to redefine the square root function so that its branch cut lies along the positive real axis. Let us take the alternative definition

$$z = |z|\,\exp(\mathrm{i}\varphi)\,, \qquad 0 \le \varphi < 2\pi\,, \qquad z^{1/2} \equiv \sqrt{|z|}\,\exp(\mathrm{i}\varphi/2)\,, \qquad 0 \le \tfrac{1}{2}\varphi < \pi\,. \tag{2.110}$$

In this case, the alternative square root is denoted as $z^{1/2}$, for reasons of avoiding an ambiguity of the notation.

With the definition (2.110), one has a situation where the sign of the square root changes as one crosses the positive real axis, i.e.,

$$\lim_{\epsilon\to 0^+} \sqrt{4+\mathrm{i}\epsilon} = 2\,, \qquad \lim_{\epsilon\to 0^+} \sqrt{4-\mathrm{i}\epsilon} = -2\,, \tag{2.111}$$

The function $z^{1/2}$ is an analytic function in the cut plane, with the branch cut along the *positive* real axis. The alternative complex square root $z^{1/2}$ has a positive imaginary part everywhere in the complex plane, $\operatorname{Im} z^{1/2} \ge 0$.

A significance is as follows. With the alternative square root function, it is possible to evaluate integrals such as

$$I' = \int_{C'} \mathrm{d}z \frac{z^{1/2}}{z^2+1}\,, \tag{2.112}$$

where C' goes infinitesimally above the negative real axis from ∞ to zero, and infinitesimally below the real axis from 0 to ∞ (see Fig. 2.4). The integral I' could not, in principle, be evaluated using the ordinary square root function, because one needs an integrand which is analytic all along the integration contour. With the ordinary definition of the square root, one would otherwise wrongfully cross the branch cut which would otherwise lie along the negative real axis.

An alternative way to evaluate the integral is as follows. One has

$$R_1' = \operatorname*{Res}_{z=\mathrm{i}} \frac{z^{1/2}}{z^2+1} = -\frac{\mathrm{i}}{2}\exp\left(\frac{1}{4}\mathrm{i}\pi\right)\,, \tag{2.113}$$

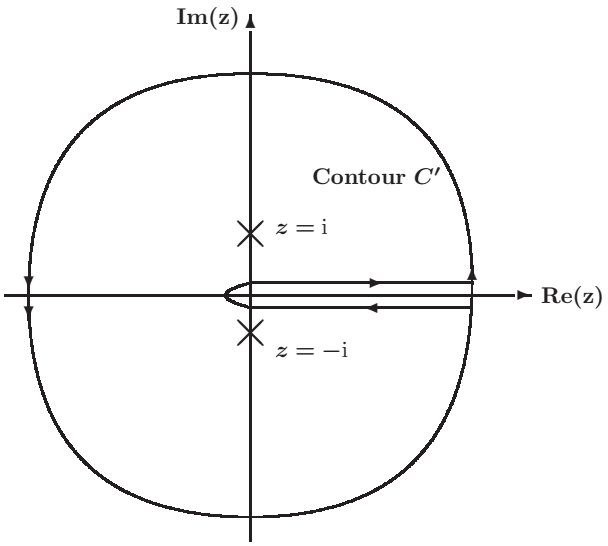

Figure 2.4: Contour C' for the integral I' given in Eq. (2.112).

while

$$R_2' = \operatorname*{Res}_{z=-\mathrm{i}} \frac{\sqrt{z}}{z^2+1} = \frac{\mathrm{i}}{2} \exp\left(\frac{3}{4}\mathrm{i}\pi\right) . \tag{2.114}$$

The sum of the residues is, with details being left to the reader to show,

$$\begin{aligned} I' &= 2\pi\mathrm{i}(R_1' + R_2') = 2\pi\mathrm{i}\left[-\frac{\mathrm{i}}{2}\exp\left(\frac{1}{4}\mathrm{i}\pi\right) + \frac{\mathrm{i}}{2}\exp\left(\frac{3}{4}\mathrm{i}\pi\right)\right] \\ &= 2\pi\mathrm{i}\left[\frac{1}{\sqrt{2}}\left(\frac{1}{2}-\frac{\mathrm{i}}{2}\right) - \frac{1}{\sqrt{2}}\left(\frac{1}{2}+\frac{\mathrm{i}}{2}\right)\right] = 2\pi\mathrm{i}\left(-\frac{\mathrm{i}}{\sqrt{2}}\right) = \sqrt{2}\pi\,. \end{aligned} \tag{2.115}$$

With the branch cuts, one obtains

$$I' = \int_{C'} \mathrm{d}z \frac{z^{1/2}}{z^2+1} = 2\int_0^\infty \mathrm{d}x \frac{2\sqrt{x}}{x^2+1} = \sqrt{2}\pi\,. \tag{2.116}$$

The definition (2.110) is relevant for the mixed frequency-coordinate-space representation of the photon Feynman propagator in quantum electrodynamics.

2.3.4 Dispersion Relations

In many cases, one can actually relate the complex contour integral around a branch cut to particular values of a complex function at a reference point in the complex plane. Applications the resulting relations, which are referred to as "dispersion relations" are numerous. Some examples come from quantum field theory, where in typical cases, the value of a complex function "on the cut" is much easier to calculate than the function itself at a particular reference point.

Side remark I: For example, in the calculation of so-called hadronic vacuum polarization, which is a fundamental process in quantum field theory that affects the photon propagator at high energies, the value of the hadronic vacuum polarization "on the cut" is related to the probability of a so-called virtual photon splitting

into hadrons. This process is much easier to calculate, and measure, than the vacuum polarization factor itself. Using a dispersion relation, one can relate the two and calculate the hadronic vacuum-polarization contribution consistently.

Side remark II: You will encounter other kinds of dispersion relations in classical electrodynamics, when you study the so-called Kramers–Kronig relations. These different dispersion relations can be derived based on certain properties of the so-called dielectric function of the material in question (the "dielectric function" describes the properties of a material as it interacts with light).

Let us study dispersion relations by way of example. With reference to Eq. (2.105), we consider the function

$$f(s) = \frac{\sqrt{s}}{s^2+1}\,, \qquad s \notin -\mathbb{R}_+. \tag{2.117}$$

We study the integral

$$J(z) = \frac{1}{2\pi\mathrm{i}} \int_C \mathrm{d}s\, \frac{f(s)}{s-z}\,, \qquad z \notin \{-\mathrm{i}, \mathrm{i}, -\mathbb{R}_+\}\,, \tag{2.118}$$

where the contour C is the same as the one that had been used for the integral I defined in Eq. (2.105). The integral $J(z)$ depends on the independent variable z, while s is the integration variable.

In the evaluation of $J(z)$, if we use residue calculus, three poles need to be considered. One of them, at $s = z$, leads to the term $f(z)$, while the others are at the isolated poles located at $s = \pm\mathrm{i}$. One has

$$J(z) = f(z) + \operatorname*{Res}_{s=-\mathrm{i}} \frac{f(s)}{s-z} + \operatorname*{Res}_{s=\mathrm{i}} \frac{f(s)}{s-z}\,, \tag{2.119}$$

On the other hand, we can also regard $J(z)$ as an explicit contour integral. Since $f(s)$ falls off sufficiently fast at large complex argument that the large circle does not contribute. Hence, alternatively, we can write

$$J(z) = \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{0} \mathrm{d}s\, \frac{f(s+\mathrm{i}\epsilon) - f(s-\mathrm{i}\epsilon)}{s-z}\,, \tag{2.120}$$

Comparing Eqs. (2.119) and (2.120), one obtains the dispersion relation

$$\begin{aligned} f(z) =& -\operatorname*{Res}_{s=-\mathrm{i}} \frac{f(s)}{s-z} - \operatorname*{Res}_{s=\mathrm{i}} \frac{f(s)}{s-z} + \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{0} \mathrm{d}s\, \frac{f(s+\mathrm{i}\epsilon) - f(s-\mathrm{i}\epsilon)}{s-z} \\ =& -\operatorname*{Res}_{s=-\mathrm{i}} \frac{f(s)}{s-z} - \operatorname*{Res}_{s=\mathrm{i}} \frac{f(s)}{s-z} + \frac{1}{\pi} \int_{-\infty}^{0} \mathrm{d}s\, \frac{\mathrm{Im} f(s+\mathrm{i}\epsilon)}{s-z}\,. \end{aligned} \tag{2.121}$$

Let us add a cryptic remark. In quantum field theory, $\mathrm{Im} f(s+\mathrm{i}\epsilon)$ might be related to a process where a virtual photon splits into a hadronic jet, while $f(z)$ might represent the hadronic vacuum-polarization contribution to the photon propagator.

It is left as an exercise for the reader to show that

$$F_1 = -\operatorname*{Res}_{s=-\mathrm{i}} \frac{f(s)}{s-z} - \operatorname*{Res}_{s=\mathrm{i}} \frac{f(s)}{s-z} = \frac{1+z}{\sqrt{2}\,(1+z^2)}\,. \tag{2.122}$$

The term from the branch cut is

$$F_2 = \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{0} \mathrm{d}s\, \frac{f(s+\mathrm{i}\epsilon) - f(s-\mathrm{i}\epsilon)}{s-z} = -\frac{1}{2\pi\mathrm{i}} \int_{0}^{\infty} \mathrm{d}t\, \frac{f(-t+\mathrm{i}\epsilon) - f(-t-\mathrm{i}\epsilon)}{-t-z} = -\frac{1}{2\sqrt{z} + \sqrt{2}\,(1+z)}\,. \tag{2.123}$$

Adding F_1 and F_2, one obtains back $f(z)$,

$$f(z) = F_1 + F_2\,. \tag{2.124}$$

The intermediate steps are left as an exercise to the reader.

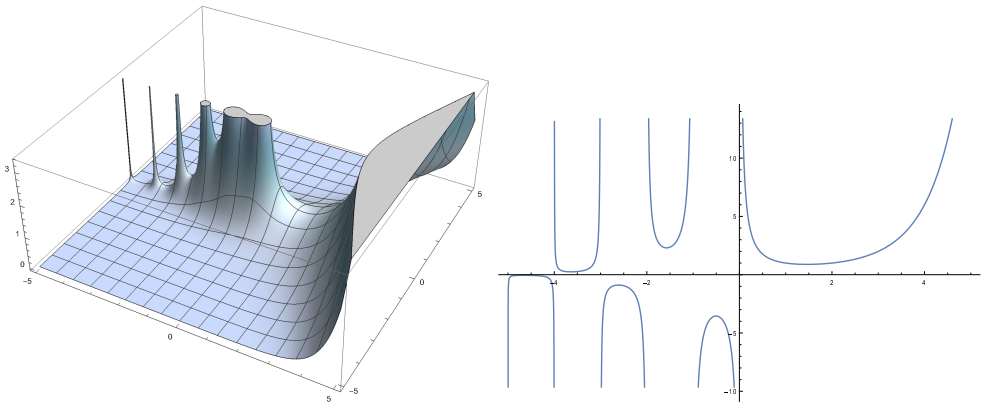

Figure 2.5: The left plot shows the modulus of the Γ in the complex plane, $f(x,y) = |\Gamma(x+\mathrm{i}y)|$. The right plot shows $f(x) = \Gamma(x)$ on the real axis.

2.3.5 Branch Cuts and Special Functions

In some cases, complex contour integrals can lead to the meromorphic continuation of a function, originally defined for real argument, into the entire complex plane (up to singular points).

One particularly instructive example is the Γ (Gamma) function, which, for positive real argument x, is given as

$$\Gamma(x) = \int_0^\infty \mathrm{d}t\, t^{x-1}\, \exp(-t)\, \mathrm{d}t\,, \qquad x > 0. \tag{2.125}$$

For $x \leq 0$, the Γ function cannot be defined by the above integral representation because of divergences incurred near $t = 0$. The recursion relation is easily shown by integration,

$$\begin{aligned}
\Gamma(x+1) &= \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-t}\, t^x\, \mathrm{d}t \\
&= \left[\mathrm{e}^{-t}\, t^x\right]_{t=0}^{t=\infty} - \int_0^\infty \mathrm{d}t\, \left(-\mathrm{e}^{-t}\right) \left(\frac{\mathrm{d}}{\mathrm{d}t} t^x\right) \mathrm{d}t \\
&= \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-t}\, \left(x\, t^{x-1}\right) \mathrm{d}t = x\, \Gamma(x)\,.
\end{aligned} \tag{2.126}$$

For a number of applications, though, one needs the Γ function (and other special functions) for complex rather than real argument. One thus needs to find the meromorphic continuation of Eq. (2.125) for complex argument.

Let us consider the complex contour integral

$$K = \int_{-\infty}^{(0^+)} \mathrm{e}^s\, s^{-z}\, \mathrm{d}s = \int_{C_0} \mathrm{e}^s\, s^{-z}\, \mathrm{d}s\,. \tag{2.127}$$

The contour C_0 starts at $z = -\infty - \mathrm{i}\epsilon$, encircles the origin in the positive sense, and ends at $z = -\infty + \mathrm{i}\epsilon$. One could thus alternatively consider the contour as

$$-\infty - \mathrm{i}\epsilon \;\to\; -\mathrm{i}\epsilon \to \text{ half-circle around origin } \to \mathrm{i}\epsilon \;\to -\infty + \mathrm{i}\epsilon\,. \tag{2.128}$$

This contour leads to a nontrivial result because the function

$$s^{-z} = \exp[-z \ln(s)] \tag{2.129}$$

has a branch cut along the negative real axis,

$$\lim_{\epsilon \to 0^+} \ln(-t + \mathrm{i}\epsilon) = \ln(|t|) + \mathrm{i}\pi\,, \qquad \lim_{\epsilon \to 0^+} \ln(-t - \mathrm{i}\epsilon) = \ln(|t|) - \mathrm{i}\pi\,, \qquad t > 0\,. \tag{2.130}$$

We can parameterize the upper part of the contour as follows,

$$s = s(t) = -t + \mathrm{i}\epsilon\,, \qquad t > 0\,. \tag{2.131}$$

We can also parameterize the upper part of the contour as follows,

$$s = s(t) = -t - \mathrm{i}\epsilon\,, \qquad t > 0\,. \tag{2.132}$$

Because the contour C_0 encircles the origin in the positive sense, the lower part of the contour is being taken in the positive sense, while the upper contour is swept backwars,

$$\begin{aligned}
K &= \int_{-\infty}^{0} \exp(-|t|)\, \exp[-z(\ln(|t|) - \mathrm{i}\pi)]\, (-1)\mathrm{d}t - \int_{-\infty}^{0} \exp(-|t|)\, \exp[-z(\ln(|t|) + \mathrm{i}\pi)]\, (-1)\mathrm{d}t \\
&= \int_{0}^{\infty} \exp(-t)\, \exp[-z(\ln(t) - \mathrm{i}\pi)]\, \mathrm{d}t - \int_{0}^{\infty} \exp(-t)\, \exp[-z(\ln(t) + \mathrm{i}\pi)]\, \mathrm{d}t \\
&= \int_{0}^{\infty} \exp(-t)\, t^{-z}\, \exp(\mathrm{i}\pi z)\, \mathrm{d}t - \int_{0}^{\infty} \exp(-t)\, t^{-z}\, \exp(-\mathrm{i}\pi z)\, \mathrm{d}t \\
&= [\exp(\mathrm{i}\pi z) - \exp(-\mathrm{i}\pi z)] \int_{0}^{\infty} \exp(-t)\, t^{-z}\, \mathrm{d}t \\
&= 2\,\mathrm{i} \sin(\pi z)\, \Gamma(1 - z)\,.
\end{aligned} \tag{2.133}$$

This consideration allows up to continue the Γ function into the complex plane, away from the real axis. We have shown the relationship

$$\int_{-\infty}^{(0^+)} \mathrm{e}^{s}\, s^{-z}\, \mathrm{d}s = 2\,\mathrm{i} \sin(\pi z)\, \Gamma(1 - z)\,, \tag{2.134}$$

which can easily be solve for $\Gamma(z)$ and serves to continue the Γ function into the complex plane (see also Fig. 2.5).

Chapter 3

Differential Equations and Green Functions

3.1 Green Functions: Different Perspectives

Let us illustrate some different perspectives. Green functions can be used for a number of different purposes, among which there are the following assignments.

- Green functions can be used as auxiliary devices in the solution of differential equations.
- Green functions represent, in some sense, superposition devices relating cause and effect.
- Green functions constitute, under certain conditions, the inverse of the kinectic (or other linear differential) operator.

Green functions are very versatile. They can be defined with having different boundary conditions in mind.

3.2 Green Function of the Harmonic Oscillator

3.2.1 Paradigmatic Equations

We shall study Green functions by way of example, and one of the most prominent and intuitive examples is that of the Green function of the damped harmonic oscillator. We shall derive some paradigmatic equations, which have widespread applicability in physical theory. In this context, it is very instructive to verify the general concept on which a Green function is based, in terms of a few basic, illustrative equations related to a damped, harmonic oscillator. Let L be a linear differential operator, an example being

$$L = \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + \gamma\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\,. \tag{3.1}$$

One way in which Green functions are useful is in the solution of inhomogeneous differential equations. Let us consider the differential equation

$$L\,x(t) = f(t) \tag{3.2}$$

with a general force term $f = f(t)$. Of course, L has the physical interpretation of the differential operator for a damped harmonic motion with an additional external perturbation $f(t)$. The variable t can be interpreted as the time.

Under this interpretation, the differential equation (3.2) can be rewritten as

$$L\,x(t) = \ddot{x}(t) + \gamma\,\dot{x}(t) + \omega_0^2\,x(t) = f(t)\,. \tag{3.3}$$

This is exactly the equation of motion expected for a classical particle in a harmonic potential, with a damping term $\gamma\,\dot{x}(t)$ and a harmonic term $\omega_0^2\,x(t)$.

Let us consider, instead of Eq. (3.2), the equation

$$L\,g(t-t') = \delta(t-t')\,, \tag{3.4}$$

where $\delta(t-t')$ is the Dirac-δ function at argument $t-t'$. One can easily show that, in this case, the expression

$$x(t) = \int_{-\infty}^{\infty} \mathrm{d}t'\,g(t-t')\,f(t') = (g\otimes f)(t)\,, \tag{3.5a}$$

$$x(t) = \textbf{Effect/Signal}\,, \tag{3.5b}$$

$$f(t) = \textbf{Cause/Source}\,, \tag{3.5c}$$

$$g(t) = \textbf{Intermediary/Auxiliary Device in Solving Eq. } (3.3)\,, \tag{3.5d}$$

solves Eq. (3.2). Here, the $\otimes$ symbol denotes the so-called convolution of functions. The convolution $(g\otimes f)(t)$ of two functions g and f at argument t is defined as $\int \mathrm{d}t'\,g(t-t')\,f(t')$. All integration intervals are maximum unless stated otherwise. We apply the differential operator L to $(g\otimes f)(t)$, with the result

$$L\,x(t) = \int_{-\infty}^{\infty} \mathrm{d}t'\,L\,g(t-t')\,f(t') = \int_{-\infty}^{\infty} \mathrm{d}t'\,\delta(t-t')\,f(t') = f(t)\,. \tag{3.6}$$

These relations illustrate why Green functions can both be regarded as auxiliary devices in the solution of differential equations, but also, as weighting factors relating cause and effect.

But why are Green functions related to the inverse of kinetic operators? Let us transform Eq. (3.4) into Fourier space,

$$L = \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + \gamma\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\,, \qquad L\,g(t-t') = \delta(t-t')\,, \tag{3.7}$$

Now,

$$\left[\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + \gamma\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\right]\,g(t-t') = \delta(t-t')\,, \tag{3.8}$$

and we have

$$\ddot{g}(\tau) + \gamma\dot{g}(\tau) + \omega_0^2\,g(\tau) = \delta(\tau)\,, \tag{3.9}$$

Now,

$$\int \mathrm{d}\tau\,\left[\ddot{g}(\tau) + \gamma\dot{g}(\tau) + \omega_0^2\,g(\tau)\right]\,\mathrm{e}^{\mathrm{i}\omega\tau} = \int \mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega\tau}\,\delta(\tau) = 1\,, \tag{3.10}$$

The integral interval is maximum. Single, and double, integrations by parts lead to

$$\int \mathrm{d}\tau\,\left[-\omega^2 g(\tau) - \mathrm{i}\gamma\omega g(\tau) + \omega_0^2\,g(\tau)\right]\,\mathrm{e}^{\mathrm{i}\omega\tau} = \int \mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega\tau}\,\delta(\tau) = 1\,. \tag{3.11}$$

This is solved by

$$\left(-\omega^2 - \mathrm{i}\gamma\omega + \omega_0^2\right) \int \mathrm{d}\tau\, g(\tau)\, \mathrm{e}^{\mathrm{i}\omega\tau} = \left(-\omega^2 - \mathrm{i}\gamma\omega + \omega_0^2\right)\, g(\omega) = 1\,. \tag{3.12}$$

So, the Green function is obtained as the inverse of the kinetic operator $-\omega^2 - \mathrm{i}\gamma\omega + \omega_0^2$, in view of the Fourier transform of the Dirac-δ being *unity* on the right-hand side of the equation. One obtains

$$g(\omega) = \frac{1}{-\omega^2 - \mathrm{i}\gamma\omega + \omega_0^2} = [-\omega^2 - \mathrm{i}\gamma\omega + \omega_0^2]^{-1}\,. \tag{3.13}$$

Again, the operator

$$\mathcal{L} = -\omega^2 - \mathrm{i}\gamma\omega + \omega_0^2 \tag{3.14}$$

can be regarded as the inverse of the operator defined in Eq. (3.7),

$$L = \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + \gamma\,\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\,, \tag{3.15}$$

in Fourier space. The fact that

$$g(\omega) = \mathcal{L}^{-1} \tag{3.16}$$

illustrates that the Green function can be regarded as the **inverse of the kinetic operator, or, linear differential operator** L. The fact that the inverse of the linear differential operator has poles, and that it is a question of how to encircle them, highlights the need to devise a specific integration prescription.

3.2.2 Green Function and Boundary Conditions

Now for the different boundary conditions. It is instructive to reconsider the defining equation of the Green function for a vanishing right-hand side $\delta\,(t-t') = 0$ and $\omega_0 = 0$,

$$\ddot{g}\,(t-t') + \gamma\,\dot{g}\,(t-t') = 0\,, \qquad g\,(t-t') = a + b\,\mathrm{e}^{-\gamma(t-t')}\,. \tag{3.17}$$

Here, a and b are integration constants. If $\gamma > 0$, then this solution is regular for $t - t' \to +\infty$ but grows exponentially for $t - t' \to -\infty$. We write the Green function as a Fourier transform

$$g(t-t') = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\,\mathrm{e}^{-\mathrm{i}\omega(t-t')}\,g(\omega) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\,\mathrm{e}^{-\mathrm{i}\omega(t-t')}\,\frac{1}{\omega_0^2 - \omega^2 - \mathrm{i}\gamma\omega}\,. \tag{3.18}$$

Now, the propagator denominator can be written in terms of a product $(\omega - \omega_1)\,(\omega - \omega_2)$,

$$g(\omega) = \frac{1}{\omega_0^2 - \omega^2 - \mathrm{i}\,\gamma\,\omega} = -\frac{1}{\omega^2 + \mathrm{i}\,\gamma\,\omega - \omega_0^2} = -\frac{1}{(\omega-\omega_1)\,(\omega-\omega_2)}\,. \tag{3.19}$$

The poles are found at

$$\omega_1 = \frac{1}{2}\,\left(-\sqrt{4\,\omega_0^2 - \gamma^2} - \mathrm{i}\,\gamma\right)\,, \qquad \omega_2 = \frac{1}{2}\,\left(\sqrt{4\,\omega_0^2 - \gamma^2} - \mathrm{i}\,\gamma\right)\,. \tag{3.20}$$

For $4\omega_0^2 > \gamma^2$, both of these poles manifestly have a negative imaginary part. One can show that

$$\operatorname*{Res}_{\omega=\omega_1}\left(-\frac{\mathrm{e}^{-\mathrm{i}\omega(t-t')}}{\omega^2 + \mathrm{i}\,\gamma\,\omega - \omega_0^2}\right) = \frac{\mathrm{e}^{-\gamma(t-t')/2}}{\sqrt{4\,\omega_0^2 - \gamma^2}}\,\exp\left[-\frac{\mathrm{i}}{2}\,\sqrt{4\,\omega_0^2 - \gamma^2}\,(t-t')\right]\,, \tag{3.21}$$

$$\operatorname*{Res}_{\omega=\omega_2}\left(-\frac{\mathrm{e}^{-\mathrm{i}\omega(t-t')}}{\omega^2 + \mathrm{i}\,\gamma\,\omega - \omega_0^2}\right) = -\frac{\mathrm{e}^{-\gamma(t-t')/2}}{\sqrt{4\,\omega_0^2 - \gamma^2}}\,\exp\left[\frac{\mathrm{i}}{2}\,\sqrt{4\,\omega_0^2 - \gamma^2}\,(t-t')\right]\,. \tag{3.22}$$

One closes the contour in Eq. (3.18) in the lower half of the complex plane, as dictated by the asymptotic behavior of the integrand, and shows that

$$g(t-t') = 2\,\Theta(t-t')\,\mathrm{e}^{-\gamma(t-t')/2}\,\frac{\sin\left(\frac{1}{2}\,\sqrt{4\omega_0^2-\gamma^2}\,(t-t')\right)}{\sqrt{4\omega_0^2-\gamma^2}}\,. \tag{3.23}$$

This Green function is a **retarded** Green function in the sense that it vanishes for $t < t'$. It still fulfills Eq. (3.8), which we recall as follows,

$$\ddot{g}\,(t-t') + \gamma\,\dot{g}\,(t-t') + \omega_0^2\,g\,(t-t') = \delta\,(t-t')\,. \tag{3.24}$$

Now, one may ask for **boundary conditions**. If $\gamma > 0$, then the limit of $g(t-t')$ as given in Eq. (3.23) is

$$g_R(t-t') = \lim_{\gamma\to 0^+} g(t-t') = 2\,\Theta(t-t')\,\frac{\sin\left(\omega_0\,(t-t')\right)}{2\omega_0} = \Theta(t-t')\,\frac{\sin\left(\omega_0\,(t-t')\right)}{\omega_0}\,. \tag{3.25}$$

However, one may convince oneself that

$$g_A(t-t') = \lim_{\gamma\to 0^-} g(t-t') = \Theta(-(t-t'))\,\frac{\sin\left(\omega_0\,[-(t-t')]\right)}{\omega_0} = \Theta(t'-t)\,\frac{\sin\left(\omega_0\,(t'-t)\right)}{\omega_0}\,. \tag{3.26}$$

This is different from the retarded Green function (3.25) by the replacement $t-t' \to t'-t$. The fact that $g_A(t-t')$ fulfills the defining equation of the Green function can be shown as follows. Let us consider a general function $g(\cdot)$ where $\tau = t-t'$, taken at negative argument $-\tau$, and let us denote the derivative function with respect to τ by a dot. One obtains

$$\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}g(-\tau) = \frac{\mathrm{d}}{\mathrm{d}\tau}(-\dot{g})(-\tau) = \ddot{g}(-\tau)\,. \tag{3.27}$$

So, if

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \omega_0^2\right)\,g(\tau) = \delta(\tau)\,, \tag{3.28}$$

then

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \omega_0^2\right)\,g(-\tau) = \delta(-\tau)\,. \tag{3.29}$$

Using the symmetry of the Dirac-δ function, one shows that the function $g(-\tau)$ fulfills the defining equation for the Green function of the undamped harmonic oscillator.

The Green function given in Eq. (3.25) is known as the **retarded** Green function, the one in Eq. (3.26) as the **advanced** Green function. Both of them fulfill the defining equation

$$\ddot{g}\,(t-t') + \omega_0^2\,g\,(t-t') = \delta(t-t')\,. \tag{3.30}$$

They still fulfill different **boundary conditions, in the sense that the retarded Green function vanishes for negative argument, while the advanced Green function vanishes for positive argument.**

The difference $g_R - g_A$ fulfills the homogeneous equation,

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \omega_0^2\right)\,[g_R(t-t') - g_A(t-t')] = 0\,. \tag{3.31}$$

This illustrates that, to any Green function, one may add (in the sense of the replacement $g \to g+h$) a solution of the homogeneous equation $L\,h = 0$.

3.2.3 Solution of Boundary–Value Problem

Let us return to the linear differential operator describing the damped driven oscillator,

$$L = \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + \gamma\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\,, \tag{3.32}$$

with the differential equation

$$L\,x(t) = \ddot{x}(t) + \gamma\,\dot{x}(t) + \omega_0^2\,x(t) = f(t)\,. \tag{3.33}$$

The Green function is given in Eq. (3.18),

$$g(t-t') = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\,\mathrm{e}^{-\mathrm{i}\omega(t-t')}\,g(\omega) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\,\mathrm{e}^{-\mathrm{i}\omega(t-t')}\,\frac{1}{\omega_0^2-\omega^2-\mathrm{i}\gamma\omega}\,. \tag{3.34}$$

We now investigate the force term

$$f\,(t') = f_0\,\Theta\,(t') + f_0\,\Theta\,(-t')\;\exp\,(t'/\tau) = f_1(t') + f_2(t')\,, \tag{3.35a}$$

$$f_1(t') = f_0\,\Theta\,(t')\;, \tag{3.35b}$$

$$f_2(t') = f_0\,\Theta\,(-t')\;\exp\,(t'/\tau)\;, \tag{3.35c}$$

and write

$$x(t) = \int_{-\infty}^{\infty}\mathrm{d}t'\,g_R(t-t')\,f(t') = x_1(t) + x_2(t)\,, \tag{3.36a}$$

$$x_1(t) = \int_{-\infty}^{\infty}\mathrm{d}t'\,g_R(t-t')\,f_1(t') = f_0\int_0^{\infty}\mathrm{d}t'\,g_R(t-t')\,, \tag{3.36b}$$

$$x_2(t) = \int_{-\infty}^{\infty}\mathrm{d}t'\,g_R(t-t')\,f_2(t') = f_0\int_{-\infty}^{0}\mathrm{d}t'\,g_R(t-t')\,\exp\,(t'/\tau)\;. \tag{3.36c}$$

Term $x_1(t)$: Let us first consider the term $x_1(t)$. From Eq. (3.36b), we see that because $g_R(t-t')$ is proportional to $\Theta(t-t')$, the whole term $x_1(t)$ vanishes for $t<0$. Otherwise, for given t, the t' integration interval is reduced to $(0,t)$. An explicit calculation (your task!) shows that

$$x_1(t) = \Theta(t)\,\frac{f_0}{\omega_0^2}\left[1-\mathrm{e}^{-\gamma t/2}\left(\cos\left(\frac{1}{2}\sqrt{4\omega_0^2-\gamma^2}\,t\right)+\gamma\,\frac{\sin\left(\frac{1}{2}\sqrt{4\omega_0^2-\gamma^2}\,t\right)}{\sqrt{4\omega_0^2-\gamma^2}}\right)\right]\,, \tag{3.37}$$

which means that the damped oscillator approaches its final position f_0/ω_0^2 at $t\to\infty$ via an exponentially damped oscillatory motion. Please note the integrals

$$\int\exp(-a\,t)\,\sin(t)\,\mathrm{d}t = -\frac{1}{a^2+1}\,\exp(-a\,t)\,[\cos(t)+a\,\sin(t)]\,, \tag{3.38a}$$

$$\int\exp(-a\,t)\,\cos(t)\,\mathrm{d}t = -\frac{1}{a^2+1}\,\exp(-a\,t)\,[-a\,\cos(t)+\sin(t)]\,. \tag{3.38b}$$

Term $x_2(t)$: For the term $x_2(t)$, we again have to differentiate two cases. If $t<0$, then the integration interval in Eq. (3.36c) is restricted to $t'\in(-\infty,t)$. If $t>0$, then the integration interval is $t'\in(-\infty,0)$.

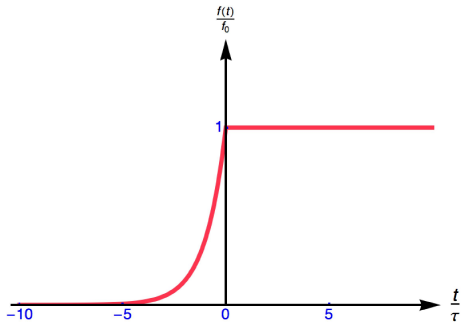

Figure 3.1: Illustration of the time-dependent force term for the harmonic oscillator, $f\,(t) = f_0\,[\Theta\,(t) + \Theta\,(-t)\exp\,(t/\tau)]$.

Hence, an explicit calculation shows that

$$x_2(t) = \Theta(t)\,\frac{\mathrm{e}^{-\gamma t/2}\,f_0\,\tau\,\left[\tau\,\sqrt{4\omega_0^2-\gamma^2}\,\cos\left(\frac{1}{2}\sqrt{4\omega_0^2-\gamma^2}\,t\right)+(2+\gamma\,\tau)\,\sin\left(\frac{1}{2}\sqrt{4\omega_0^2-\gamma^2}\,t\right)\right]}{\sqrt{4\omega_0^2-\gamma^2}\,(1+\tau\,(\gamma+\tau\,\omega_0^2))}$$
$$+\,\Theta(-t)\,\frac{\mathrm{e}^{t/\tau}\,f_0\,\tau^2}{1+\tau\,(\gamma+\tau\,\omega_0^2)}\,. \tag{3.39}$$

The full solution can then be presented as

$$x(t) = \Theta(t)\,f_0\,\left(\frac{1}{\omega_0^2}-\frac{\mathrm{e}^{-\gamma t/2}\,(1+\gamma\tau)\,\cos\left(\frac{1}{2}\sqrt{4\omega_0^2-\gamma^2}\,t\right)}{\omega_0^2(1+\gamma\tau+\tau^2\,\omega_0^2)}\right.$$
$$\left.-\frac{\mathrm{e}^{-\gamma t/2}\,(\gamma+\gamma^2\,\tau-2\omega_0^2\tau)\,\sin\left(\frac{1}{2}\sqrt{4\omega_0^2-\gamma^2}\,t\right)}{\omega_0^2\,\sqrt{4\omega_0^2-\gamma^2}\,(1+\gamma\tau\,+\omega_0^2\tau^2)}\right)+\Theta(-t)\,\frac{f_0\,\mathrm{e}^{t/\tau}\,\tau^2}{1+\tau\,(\gamma+\tau\,\omega_0^2)}$$
$$=\Theta(t)\,x_+(t)+\Theta(-t)\,x_-(t)\,. \tag{3.40}$$

It fulfills

$$x(t)\to 0 \quad \text{for} \quad t\to-\infty\,, \qquad x(t)\to\frac{f_0}{\omega_0^2} \quad \text{for} \quad t\to+\infty\,. \tag{3.41}$$

This is consistent with the boundary conditions naturally fulfilled by the retarded Green function, namely, vanishing boundary conditions in the infinite past. At $t=0$, the two terms are in agreement at

$$x(0)=\frac{f_0\,\tau^2}{1+\gamma\,\tau+\omega_0^2\tau^2}\,. \tag{3.42}$$

The work done on the oscillator is

$$W=\int\vec{f}\,\cdot\,\mathrm{d}\vec{s}=\int_{-\infty}^{\infty}f(t)\,\dot{x}(t)\,\mathrm{d}t=\int_0^{\infty}f(t)\,\dot{x}_+(t)\,\mathrm{d}t+\int_{-\infty}^{0}f(t)\,\dot{x}_-(t)\,\mathrm{d}t$$
$$=\frac{f_0^2\tau^2}{2+2\gamma\,\tau+2\tau^2\,\omega_0^2}+\frac{f_0^2\,(1+\gamma\,\tau)}{\omega_0^2\,[1+\tau(\gamma+\omega_0^2\tau)]}=\frac{f_0^2}{\omega_0^2}-\frac{1}{2}\frac{f_0^2\tau^2}{1+\tau(\gamma+\omega_0^2\tau)}\,. \tag{3.43}$$

The energy stored in the harmonic oscillator is

$$E=\frac{1}{2}\,\dot{x}^2+\frac{1}{2}\,\omega_0^2x^2\,, \tag{3.44}$$

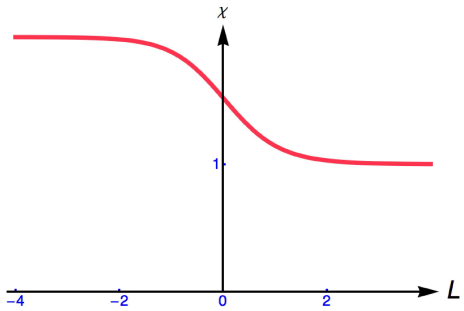

Figure 3.2: Plot of the ratio χ as defined in Eq. (3.46) for $\gamma = \omega_0/10$, with $X = \omega_0\,\tau = \exp(L)$.

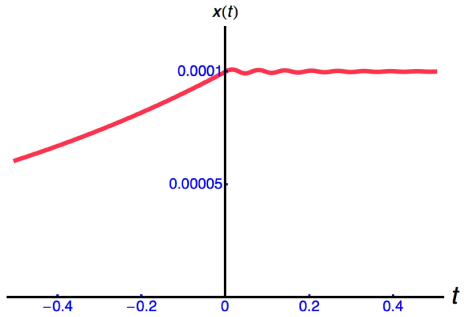

Figure 3.3: Plot of the trajectory $x(t)$ as obtained via the Green function formalism, for $\gamma = \omega_0/10$, $\omega_0 = 100$, and $\tau = 1$ as well as $f_0 = 1$.

For $t \to +\infty$, the time derivative of the trajectory $x(t)$ vanishes, and $x(t) \to f_0/\omega_0^2$. So,

$$E_\infty \to \frac{1}{2}\,\omega_0^2\,\left(\frac{f_0}{\omega_0^2}\right)^2 = \frac{1}{2}\,\frac{f_0^2}{\omega_0^2} \qquad \text{for} \qquad t \to +\infty\,. \tag{3.45}$$

The ratio is

$$\chi = \frac{W}{E_\infty} = 1 + \frac{1+\gamma\,\tau}{1+\tau(\gamma+\omega_0^2\tau)}\,. \tag{3.46}$$

For a relatively strongly damped system with $\gamma = \omega_0/10$, we have

$$\chi = 1 + \frac{10+X}{10+X+10X^2}\,, \qquad X = \omega_0\,\tau\,, \qquad \gamma = \frac{\omega_0}{10}\,. \tag{3.47}$$

Setting $X = \exp(L)$, the dependence of χ on L is shown in Fig. 3.2. If the time scale τ during which the force is being switched on, is large on the time scale of the undamped oscillation, then $X = \omega_0\,\tau \gg 1$. Also, in that case, L is large, and the motion of the harmonic oscillator is only slightly damped. So, in that case, $\chi \to 1$. If the motion is strongly damped on the time scale of the undamped oscillation, then $\chi \to 2$, and half of the work invested in driving the oscillator is wasted into the damping friction force. An example of an only slightly damped motion with $\gamma = \omega_0/10$, $\omega_0 = 100$, $\tau = 1$, thus $X = \omega_0\,\tau = 100 \gg 1$, and $f_0 = 1$ is shown in Fig. 3.3.

3.2.4 Green Function and Concatenation Approach

An alternative way of constructing the Green function is as follows. We first observe that the inhomogeneous and homogeneous equations, which we recall for convenience,

$$\frac{\mathrm{d}^2}{\mathrm{d}s^2} g\,(s) + \gamma\,\frac{\mathrm{d}}{\mathrm{d}s} g\,(s) + \omega_0^2\; g\,(s) = \delta\,(s)\;, \tag{3.48a}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}s^2} h\,(s) + \gamma\,\frac{\mathrm{d}}{\mathrm{d}s} h\,(s) + \omega_0^2\; h\,(s) = 0\,, \tag{3.48b}$$

are actually equivalent to each other except for the immediate vicinity of $s = 0$, because $\delta(s \neq 0) = 0$. Now, the general solution of the homogeneous equation can be easily determined and enters our ansatz for the Green function, which reads

$$\begin{aligned} g\,(s) = \Theta(s)\; &\left[A_+\,\mathrm{e}^{-\gamma\,s/2}\,\sin\left(\frac{1}{2}\,\sqrt{4\omega_0^2-\gamma^2}\;s\right)\right. \\ &\left.+B_+\,\mathrm{e}^{-\gamma\,s/2}\,\cos\left(\frac{1}{2}\,\sqrt{4\omega_0^2-\gamma^2}\;s\right)\right] \\ +\,\Theta(-s)\; &\left[A_-\,\mathrm{e}^{-\gamma\,s/2}\,\sin\left(\frac{1}{2}\,\sqrt{4\omega_0^2-\gamma^2}\;s\right)\right. \\ &\left.+B_-\,\mathrm{e}^{-\gamma\,s/2}\,\cos\left(\frac{1}{2}\,\sqrt{4\omega_0^2-\gamma^2}\;s\right)\right]\,. \end{aligned} \tag{3.49}$$

The integration constants $A_\pm$ and $B_\pm$ can be determined by *(i)* boundary conditions and *(ii)* integrating Eq. (3.48a) in an infinitesimal interval about $s = 0$. For the retarded Green function, we have to require that $A_- = B_- = 0$. This also follows from the regularity requirement at $s = -\infty$; the numerical value of the Green function would otherwise diverge in that limit. Furthermore, as the Green function needs to be continuous at $s = 0$, we have to impose the condition $B_+ = 0$; the cosine would otherwise induce a kink. After setting $A_- = B_- = B_+ = 0$, the remaining parameter A_+ can be determined by integrating Eq. (3.48a) in an infinitesimal interval around $s = 0$,

$$\begin{aligned} 1 &= \int_{-\epsilon}^{\epsilon} \delta\,(s)\;\mathrm{d}s = \int_{-\epsilon}^{\epsilon} \left[\frac{\mathrm{d}^2}{\mathrm{d}s^2} g\,(s) + \gamma\,\frac{\mathrm{d}}{\mathrm{d}s} g\,(s) + \omega_0^2\; g\,(s)\right]\,\mathrm{d}s \\ &= \left.\frac{\mathrm{d}}{\mathrm{d}s} g\,(s)\right|_{s=\epsilon} - \left.\frac{\mathrm{d}}{\mathrm{d}s} g\,(s)\right|_{s=-\epsilon} + \gamma\,[g(\epsilon) - g(-\epsilon)] + \omega_0^2\; g(0)\;\epsilon + \mathcal{O}(\epsilon^2) \\ &= \left.\frac{\mathrm{d}}{\mathrm{d}s} g\,(s)\right|_{s=\epsilon} - \left.\frac{\mathrm{d}}{\mathrm{d}s} g\,(s)\right|_{s=-\epsilon} + \mathcal{O}(\epsilon) = \left(\frac{1}{2}\,A_+\,\sqrt{4\,\omega_0^2-\gamma^2}\right) - (0) + \mathcal{O}(\epsilon)\,. \end{aligned} \tag{3.50}$$

We have assumed that the Green function itself is continuous while its derivative may have a kink. The result thus reads

$$A_+ = \frac{2}{\sqrt{4\,\omega_0^2-\gamma^2}}\,. \tag{3.51}$$

Inserting this result into Eq. (3.49), we recover (3.23),

$$g(s) = 2\,\Theta(s)\,\mathrm{e}^{-\gamma s/2}\,\frac{\sin\left(\frac{1}{2}\,\sqrt{4\omega_0^2-\gamma^2}\,s\right)}{\sqrt{4\omega_0^2-\gamma^2}}\,. \tag{3.52}$$

The "concatenation approach" can be used, with good effect, for the calculation of many Green functions relevant to practical applications.

3.3 Green Function of the Poisson Equation

3.3.1 Poisson Equation in Three Dimensions

Let us give two more examples. In electrostatics, one solves the Poisson equation

$$\vec{\nabla}^2 \Phi(\vec{r}) = -\frac{1}{\epsilon_0}\,\rho(\vec{r})\,, \qquad \vec{\nabla}^2 g(\vec{r}-\vec{r}') = \delta^{(3)}(\vec{r}-\vec{r}')\,. \tag{3.53}$$

Here, we denote the Green function of the Poisson equation again as g. One may easily convince oneself that

$$g(\vec{r}-\vec{r}') = -\frac{1}{4\pi}\,\frac{1}{|\vec{r}-\vec{r}'|} = \int \frac{\mathrm{d}^3 k}{(2\pi)^3}\,\frac{1}{\vec{k}^2}\,\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}}\,, \tag{3.54}$$

is a Green function of the Poisson equation, which fulfills the defining equation

$$\vec{\nabla}^2 g(\vec{r}-\vec{r}') = \delta^{(3)}(\vec{r}-\vec{r}')\,, \tag{3.55}$$

while also fulfilling boundary conditions of a vanishing Green function in the limit $|\vec{r}-\vec{r}'| \to \infty$. One particular solution to the Poisson equation can then be found as

$$\Phi(\vec{r}) = \int \mathrm{d}^3\, r'\, g(\vec{r}-\vec{r}')\,\rho(\vec{r}') = -\frac{1}{\epsilon_0}\int \mathrm{d}^3\, r'\,\frac{1}{|\vec{r}-\vec{r}'|}\,\rho(\vec{r}')\,. \tag{3.56}$$

The second representation in Eq. (3.54) illustrates the use of the Green function as the inverse of the kinetic operator, in this case, $\vec{k}^2$, while Eq. (3.56) illustrates the use of the **Green function as in intermediary "collection instrument" linking the cause, namely, the charge distribution $\rho(\vec{r})$, and the corresponding effect, namely, the electrostatic potential $\Phi(\vec{r})$.**

In fact, Green functions of the Poisson equation different from those given in Eq. (3.54) can be devised; those can be designed to fulfill specific boundary conditions on a two-dimensional subset of three-dimensional space. The corresponding boundary–value problems are known as the Dirichlet and von Neumann problems and are the subject of study in electrostatics and elsewhere.

3.3.2 Poisson Equation for General Dimension

As a last application in the current lecture, let us investigate the solution of the Poisson equation in D dimensions.

$$\vec{\nabla}^2 g(\vec{r}-\vec{r}') = \delta^{(D)}(\vec{r}-\vec{r}')\,, \tag{3.57}$$

where g is the Green function and $\vec{r}$ is the D-dimensional position vector. One possible *ansatz* in the calculation of g is to consider the integral of the gradient of $1/r^{D-2}$. One considers the D-dimensional gradient operator $\vec{\nabla}$ and the radial variable r in D dimensions,

$$\vec{\nabla} = \sum_{i=1}^{D} \hat{\mathrm{e}}_i\,\frac{\partial}{\partial x_i}\,, \qquad r = \sqrt{\sum_{j=1}^{D}(x_j)^2}\,, \tag{3.58}$$

Here, the x_i are the Cartesian coordinates in D dimensions. One shows that

$$\vec{\nabla}\frac{1}{r^{D-2}} = \left(\frac{\partial}{\partial r}\frac{1}{r^{D-2}}\right)\left(\frac{\partial r}{\partial \vec{r}}\right) = -(D-2)\,\frac{\vec{r}}{r^D}\,. \tag{3.59}$$

Also, we convince ourselves that

$$\begin{aligned}\frac{1}{D-2}\,\vec{\nabla}^2\frac{1}{r^{D-2}} =& -\vec{\nabla}\cdot\left(\frac{\vec{r}}{r^D}\right) = -\sum_{i=1}^{D}\frac{\partial}{\partial x_i}\frac{x_i}{r^D}\\ =& -\frac{1}{r^D}\sum_{i=1}^{D}\left(\frac{\partial}{\partial x_i}x_i\right) - \sum_{i=1}^{D}x_i\left(\frac{\partial}{\partial x_i}\frac{1}{r^D}\right) = -\frac{D}{r^D} - \sum_{i=1}^{D}x_i\left(-\frac{D\,x_i}{r^{D+2}}\right)\\ =& -\frac{D}{r^D} + \frac{D\,r^2}{r^{D+2}} = -\frac{D-D}{r^D} = 0\,, \qquad \vec{r}\neq\vec{0}\,. \end{aligned} \tag{3.60}$$

The *ansatz*

$$\vec{\nabla}^2\frac{1}{r^{D-2}} = -A\,\delta^{(D)}(\vec{r}) \tag{3.61}$$

is therefore justified, with a constant A which remains to be determined. It is sufficient to argue that, because the expression $\vec{\nabla}^2\,r^{-(D-2)}$ vanishes everywhere except at the origin, the result for $\vec{\nabla}^2\,r^{-(D-2)}$ has to be centered at the origin.

One denotes by S the sphere of radius $r=|\vec{r}|$ embdeded in D dimensions, and by ∂S its surface. Then, convince yourself (how?) that the vector-valued (normal pointing outward) infinitesimal surface element of the D-dimensional unit sphere is

$$\mathrm{d}\vec{A} = \hat{r}\,r^{D-1}\mathrm{d}\Omega_D = \vec{r}\,r^{D-2}\mathrm{d}\Omega_D\,, \qquad \hat{r}=\vec{r}/|\vec{r}|\,. \tag{3.62}$$

Here, $\mathrm{d}\Omega_D$ is the infinitesimal solid angle in D dimensions,

$$\Omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}\,. \tag{3.63}$$

It is a good exercise to find for illustration, a convenient representation of $\mathrm{d}\Omega_D$ in $D=2$ dimensions, in terms of an angle (which one?). Recall (which one?) a convenient representation of $\mathrm{d}\Omega_D$ in $D=3$ dimensions. One also finds, from Jentschura and Sapirstein [J. Phys. Commun. **2** (2018) 015026], a convenient representation of $\mathrm{d}\Omega_D$ in $D=4$ dimensions. Then,

$$\begin{aligned}\int_{\partial S}\left(\vec{\nabla}\frac{1}{r^{D-2}}\right)\cdot\mathrm{d}\vec{A} =& -(D-2)\int\left(\frac{\vec{r}}{r^D}\right)\cdot\left(\vec{r}\,r^{D-2}\right)\,\mathrm{d}\Omega_D = -(D_2)\int r^{-D}\,(\vec{r}\cdot\vec{r})\,r^{D-2}\mathrm{d}\Omega_D\\ =& -(D-2)\int r^{-D}r^2r^{D-2}\mathrm{d}\Omega_D = -(D-2)\int\mathrm{d}\Omega_D\\ =& -(D-2)\Omega_D = -(D-2)\frac{2\pi^{D/2}}{\Gamma(D/2)}\,. \end{aligned} \tag{3.64}$$

By using the divergence theorem, show that one has, with the help of the *ansatz* given in Eq. (3.61),

$$\int_{\partial S}\left(\vec{\nabla}\frac{1}{r^{D-2}}\right)\cdot\mathrm{d}\vec{A} = \int_S\left(\vec{\nabla}^2\frac{1}{r^{D-2}}\right)\mathrm{d}V = -A\int_S\delta^{(D)}(\vec{r})\,\mathrm{d}V = -A\,. \tag{3.65}$$

Comparing relations (3.64) and (3.65), one arrives at the result

$$\vec{\nabla}^2\frac{1}{r^{D-2}} = -A\,\delta^{(D)}(\vec{r}) = -(D-2)\,\Omega_D\,\delta^{(D)}(\vec{r}) \tag{3.66}$$

Hence, one finds the Green function of the D-dimensional Poisson equation as follows,

$$\vec{\nabla}^2 g(\vec{r}-\vec{r}') = \delta^{(D)}(\vec{r})\,, \qquad g(\vec{r}-\vec{r}') = -\frac{1}{(D-2)\Omega_D}\,\frac{1}{|\vec{r}-\vec{r}'|^{D-2}}\,, \qquad D\neq 2\,. \tag{3.67}$$

For $D = 3$, this result reproduces the familiar formula

$$g(\vec{r} - \vec{r}') = -\frac{1}{4\pi|\vec{r} - \vec{r}'|}\,, \qquad \vec{\nabla}^2 \left(-\frac{1}{4\pi|\vec{r} - \vec{r}'|}\right) = \delta^{(3)}(\vec{r} - \vec{r}')\,. \tag{3.68}$$

For $D = 4$, one has $\Omega_4 = 2\pi^2$ and $D - 2 = 2$, so that

$$g(\vec{\xi} - \vec{\xi}') = -\frac{1}{4\pi^2|\vec{\xi} - \vec{\xi}'|^2}\,, \qquad \vec{\nabla}^2 \left(-\frac{1}{4\pi^2|\vec{\xi} - \vec{\xi}'|^2}\right) = \delta^{(4)}(\vec{\xi} - \vec{\xi}')\,. \tag{3.69}$$

Here, we use $\vec{\xi}$ to denote the position vector in four dimensions. This result reproduces Eq. (35) of Jentschura and Sapirstein [J. Phys. Commun. **2** (2018) 015026].

The general result in Eq. (3.67) obviously cannot be valid for $D = 2$, because the exponent in the expression $1/|\vec{r} - \vec{r}'|^{D-2}$ vanishes. Show that, in $D = 2$, the surface ∂S constitutes the unit sphere embedded in two dimensions. I.e., it is the unit circle. The normal is pointing outward. Then, we need to solve

$$\vec{\nabla}^2 g(\vec{r}) = \delta^{(2)}(\vec{r})\,. \tag{3.70}$$

Consider an *ansatz*

$$g(\vec{r}) = A\,\ln\left(\frac{r}{a}\right)\,, \tag{3.71}$$

and calculate the gradient

$$\vec{\nabla} g(\vec{r}) = \vec{\nabla} A\,\ln\left(\frac{r}{a}\right) = A\,\frac{a}{r}\,\vec{\nabla}\left(\frac{r}{a}\right) = A\frac{1}{r}\left(\frac{\vec{r}}{r}\right) = A\frac{\vec{r}}{r^2}\,. \tag{3.72}$$

Show that the surface "area" element, in two dimensions, of the generalized "sphere" of radius r (i.e., the circle of radius r) is

$$\mathrm{d}\vec{A} = \vec{r}\,\mathrm{d}\theta\,. \tag{3.73}$$

Question to the reader: How do you interpret $\mathrm{d}\theta$ geometrically? Why do we use $\vec{r}$ and not $\hat{r}$ in this formula? One calculates the "surface area"

$$\int \hat{r}\cdot\mathrm{d}\vec{A} = \int \hat{r}\cdot\vec{r}\,\mathrm{d}\theta = r\int \mathrm{d}\theta = 2\pi r \tag{3.74}$$

which is equal to the circumference of the circle of radius r. By using the divergence theorem in two dimensions, one shows that

$$\int_S \vec{\nabla}^2 g(\vec{r})\,\mathrm{d}V = \int_{\partial S} \vec{\nabla} g(\vec{r})\cdot\mathrm{d}\vec{A} = A\int_{\partial S}\frac{\vec{r}}{r^2}\cdot\vec{r}\,\mathrm{d}\theta = 2\pi A\,. \tag{3.75}$$

Then, using the ansatz (3.71), one has

$$\int_S \vec{\nabla}^2 g(\vec{r})\mathrm{d}V = \int_S \delta^{(2)}(\vec{r})\mathrm{d}V = 1\,. \tag{3.76}$$

Hence, one shows that

$$A = \frac{1}{2\pi}\,. \tag{3.77}$$

Finally, explain why

$$\vec{\nabla}^2 g(\vec{r} - \vec{r}') = \delta^{(2)}(\vec{r})\,, \qquad g(\vec{r} - \vec{r}') = \frac{1}{2\pi}\ln\left(\frac{|\vec{r} - \vec{r}'|}{a}\right)\,, \qquad D = 2\,. \tag{3.78}$$

solves the Poisson equation in two dimensions.

Why do you obtain the result $\Omega_{D=1} = 2$ instead of one? What happens with the Poisson equation in one dimension?

We conclude these notes with some rather wonderful observations on the consistency of mathematics.

We recall the result for the Green function of the Poisson equation for general D dimensions given in Eq. (3.67),

$$G(\vec{r} - \vec{r}') = -\frac{1}{(D-2)\Omega_D} \frac{1}{|\vec{r} - \vec{r}'|^{D-2}}, \qquad D \neq 2. \tag{3.79}$$

We also recall the result in two dimensions, from Eq. (3.78),

$$G(\vec{r} - \vec{r}') = \frac{1}{2\pi} \ln\left(\frac{|\vec{r} - \vec{r}'|}{a}\right), \qquad D = 2. \tag{3.80}$$

Let us set $D = 2 + \varepsilon$ in the result for general dimension, and expand for small ε,

$$\begin{aligned} G(\vec{r} - \vec{r}') = & -\frac{1}{\varepsilon\Omega_{2+\epsilon}} \frac{1}{|\vec{r} - \vec{r}'|^{\varepsilon}} = -\frac{1}{\varepsilon\Omega_D} \frac{1}{|\vec{r} - \vec{r}'|^{\varepsilon}} \\ = & -\frac{1}{2\pi\varepsilon} + \frac{1}{4\pi} \{2\ln(|\vec{r} - \vec{r}'|) + \ln(\pi) + \gamma_E\} + \mathcal{O}(\varepsilon). \end{aligned} \tag{3.81}$$

The constant term $-\frac{1}{2\pi\varepsilon}$ has no physical consequences even though it is divergent in the limit $\varepsilon \to 0$. The same applies to the constant terms in the order ε^0. Adjusting the constant appropriately, one obtains the result for $D = 2$ in the limiting process $\epsilon \to 0^+$. We have used the replica trick given in Eq. (2.13).

3.4 Further Applications of Green Functions

3.4.1 Green Function for the Wave Equation

As a last example, for the **wave equation**. The linear operator L, the Green function G, the signal function ψ, and the source term F are related by

$$L = \epsilon_0 \left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \vec{\nabla}^2\right), \tag{3.82a}$$

$$L\, G(\vec{r} - \vec{r}', t - t') = \delta^{(3)}(\vec{r} - \vec{r}')\, \delta(t - t'), \tag{3.82b}$$

$$L\, \psi(\vec{r} - \vec{r}', t - t') = \frac{1}{\epsilon_0} F(\vec{r}, \vec{t}), \tag{3.82c}$$

$$\psi(\vec{r}, t) = \int \mathrm{d}^3 r' \int \mathrm{d}^3 t'\, G(\vec{r} - \vec{r}', t - t')\, F(\vec{r}', \vec{t}'). \tag{3.82d}$$

Here, the Green function can be a retarded or advanced, or, the so-called Feynman Green function. This is discussed by **U.D.Jentschura in Advanced Classical Electrodynamics (World Scientific, 2017).** Green functions are very powerful tools.

3.4.2 Green Function and Atomic Polarizability

Let us try to connect our formalism as developed so far, to the properties of constituent atoms in a sample, combining the wisdom learned from the analysis of a Green function, with our picture of a damped harmonic

oscillator, to see what we can learn about an atom in a sample, seen as a collection of driven damped harmonic oscillators, which describe the atomic transitions.

We will end up with a rather general model for the dielectric constant. In terms of the susceptibility $\chi_e(\omega)$, we have

$$\epsilon(\omega) = \epsilon_0\,\epsilon_r(\omega) = \epsilon_0\,\left(1+\chi_e(\omega)\right)\,, \qquad \tilde{\vec{D}}(\vec{r},\omega) = \epsilon(\omega)\,\tilde{\vec{E}}(\vec{r},\omega) = \epsilon_r(\omega)\,\epsilon_0\,\tilde{\vec{E}}(\vec{r},\omega)\,. \tag{3.83}$$

where $\epsilon_r(\omega)$ is a dimensionless relative polarizability. By definition, the dipole moment of an atom is related to its polarizability $\alpha(\omega)$ and to the applied electric field $\vec{E}(\omega)$ as follows (we assume spatially uniform fields)

$$\vec{p}_n = \sum_j q_{jn}\,\vec{r}_{jn} = \alpha(\omega)\,\vec{E}(\vec{r},\omega)\,, \tag{3.84}$$

where we assume that $\alpha(\omega)$ is taylored to the nth atom. We had defined the polarization as

$$\vec{P}(\vec{r},\omega) = \sum_n \vec{p}_n\,f(\vec{r}-\vec{r}_n) = \frac{N}{V}\vec{p}_n = \frac{N}{V}\,\alpha(\omega)\,\vec{E}(\vec{r},\omega)\,, \tag{3.85}$$

where we assume that the test function $f(\vec{r}-\vec{r}_n)$ is a unit test function for the volume V, and there are N atoms in the test volume. Note that the normalization condition $\int d^3r\,f(\vec{r}-\vec{r}_n)=1$ implies that f must have dimension of inverse volume. On the other hand,

$$\begin{aligned}\vec{D}(\vec{r},\omega) &= \epsilon_0\,\left(\vec{E}(\vec{r},\omega)+\frac{1}{\epsilon_0}\vec{P}(\vec{r},\omega)\right) = \epsilon_0\,\left(1+\frac{1}{\epsilon_0}\frac{N}{V}\,\alpha(\omega)\right)\,\vec{E}(\vec{r},\omega)\\ &= \epsilon_0\,\left(\vec{E}(\vec{r},\omega)+(\epsilon_r(\omega)-1)\,\vec{E}(\vec{r},\omega)\right)\,.\end{aligned} \tag{3.86}$$

Denoting by $\alpha(\omega)$ the dipole polarizability of the atom, we have

$$\epsilon_r(\omega)-1 = \chi_e(\omega) = \frac{N_V}{\epsilon_0}\,\alpha(\omega)\,, \qquad N_V = \frac{N}{V}\,, \tag{3.87}$$

where N_V is the volume density of atoms. By convention, $\alpha(\omega)=\alpha_{\ell=1}(\omega)$ is the dipole ($2^{\ell=1}$-pole) dynamic polarizability of the ground state $|\phi_0\rangle$ of an atom. In terms of the oscillator strength $f_{n0}=f_{n0}^{(\ell=1)}$, we have a sum over virtual excited states $|\phi_n\rangle$,

$$\alpha(\omega) = \sum_n \frac{f_{n0}}{E_{n0}^2-(\hbar\omega)^2}\,. \tag{3.88}$$

The energy differences between the ground state and the excited states are $E_{n0}=E_n-E_0$, where the sum over n also includes the continuous spectrum. The sum over n includes, in particular, all magnetic projections of the virtual states $|\phi_n\rangle$. The 2^ℓ-multipole oscillator strength is

$$f_{n0}^{(\ell)} = 2\,\frac{4\pi e^2}{(2\ell+1)^2}\,E_{n0}\,\sum_m\sum_{m_n}\left|\left\langle\,\phi_n\,\left|\sum_i (r_i)^\ell\,Y_{\ell m}(\hat{r}_i)\right|\,\phi_0\,\right\rangle\right|^2\,, \tag{3.89}$$

where we sum over the magnetic projections m of the spherical harmonic and over the magnetic projections m_n of the excited state $|\phi_n\rangle$. Furthermore, r_i is the radial coordinate of the ith electron, and $Y_{\ell m}(\hat{r}_i)$ is the spherical harmonic with the argument being equal to the unit vector of the position of the ith electron. The sum is over all electrons i whose position is $\vec{r}_i$ within the atomic system. The dipole oscillator strength is

$$f_{n0} = f_{n0}^{(\ell=1)}\,. \tag{3.90}$$

There is a sum rule,

$$\sum_n f_{n0} = Z\, e^2\, a_0^2\, E_h\,, \qquad a_0 = \frac{\hbar}{\alpha\, m_e\, c}\,, \qquad E_h = \alpha^2 m_e c^2\,. \tag{3.91}$$

Here, a_0 is the Bohr radius, E_h is the Hartree energy, and e is the elementary charge. Let us check units:

$$f_{n0} \sim (\mathrm{Cm})^2\,\mathrm{J}\,, \tag{3.92a}$$

$$\epsilon_0 \sim \frac{\mathrm{A\,s}}{\mathrm{V\,m}} = \frac{\mathrm{C}}{\mathrm{V\,m}}\,, \tag{3.92b}$$

$$\frac{N_V}{\epsilon_0}\,\frac{f_{n0}}{E_{n0}^2} \sim \frac{1}{\mathrm{m}^3}\,\frac{\mathrm{m\,V}}{\mathrm{C}}\,\frac{(\mathrm{Cm})^2}{\mathrm{J}^2}\,\mathrm{J} = \frac{\mathrm{J\,C}}{\mathrm{V}} = 1\,. \tag{3.92c}$$

We may restore the imaginary part of the virtual state energy according to

$$E_{n0} \to \mathrm{Re}\, E_{n0} + \mathrm{i}\,\mathrm{Im} E_{n0} = E_{n0} - \frac{\mathrm{i}}{2}\,\Gamma_n\,. \tag{3.93}$$

This corresponds to a spontaneous decay of the virtual state as

$$E_{n0} \to E_{n0} - \frac{\mathrm{i}}{2}\,\Gamma_n\,, \qquad \Gamma_n \ll E_{n0}\,, \tag{3.94}$$

where we have defined the Γ_n to be the imaginary part of the energy, as opposed to $\gamma_n = \Gamma_n/\hbar$, which has the physical dimension of frequency. So,

$$\left|\exp\left(-\mathrm{i}\,E_{n0}\,t\right)\right|^2 \to \left|\exp\left(-\mathrm{i}\,E_{n0}\,t - \frac{1}{2}\,\Gamma_n\,t\right)\right|^2 = \exp\left(-\Gamma_n\,t\right)\,. \tag{3.95}$$

In view of the identity

$$\frac{2E_{n0}}{E_{n0}^2 - (\hbar\omega)^2} = \frac{1}{E_{n0} - \hbar\omega} + \frac{1}{E_{n0} + \hbar\omega} \;\to\; \frac{1}{E_{n0} - \frac{\mathrm{i}}{2}\Gamma_n - \hbar\omega} + \frac{1}{E_{n0} - \frac{\mathrm{i}}{2}\Gamma_n + \hbar\omega}\,, \tag{3.96}$$

we can write $\alpha(\omega)$ as

$$\alpha(\omega) = \sum_n \frac{f_{n0}}{2E_{n0}}\left(\frac{1}{E_{n0} - \hbar\omega} + \frac{1}{E_{n0} + \hbar\omega}\right) \;\to\; \sum_n \frac{f_{n0}}{2E_{n0}}\left(\frac{1}{E_{n0} - \frac{\mathrm{i}}{2}\,\Gamma_n - \hbar\omega} + \frac{1}{E_{n0} - \frac{\mathrm{i}}{2}\,\Gamma_n + \hbar\omega}\right)\,. \tag{3.97}$$

We can approximate, neglecting terms of order Γ_n^2,

$$\frac{1}{2E_{n0}}\left(\frac{1}{E_{n0} - \mathrm{i}\frac{1}{2}\,\Gamma_n - \hbar\omega} + \frac{1}{E_{n0} - \mathrm{i}\frac{1}{2}\,\Gamma_n + \hbar\omega}\right) \approx \frac{1}{\left(E_{n0} - \mathrm{i}\frac{1}{2}\,\Gamma_n\right)^2 - (\hbar\omega)^2}\,. \tag{3.98}$$

Furthermore,

$$\frac{1}{\left(E_{n0} - \mathrm{i}\frac{1}{2}\,\Gamma_n\right)^2 - (\hbar\omega)^2} \approx \frac{1}{E_{n0}^2 - \mathrm{i}\,\Gamma_n\; E_{n0} - (\hbar\omega)^2} \approx \frac{1}{E_{n0}^2 - \mathrm{i}\,\Gamma_n\;\hbar\,\omega - (\hbar\omega)^2}\,. \tag{3.99}$$

The modification due to Γ_n is important only in the vicinity of the resonance. The corresponding expression for $\alpha(\omega)$ is the **Atomic Polarizability as a Sum over Harmonic Oscillators:**

$$\alpha(\omega) = \sum_n \frac{f_{n0}}{E_{n0}^2 - \mathrm{i}\,\Gamma_n\;\hbar\,\omega - (\hbar\omega)^2}\,. \tag{3.100}$$

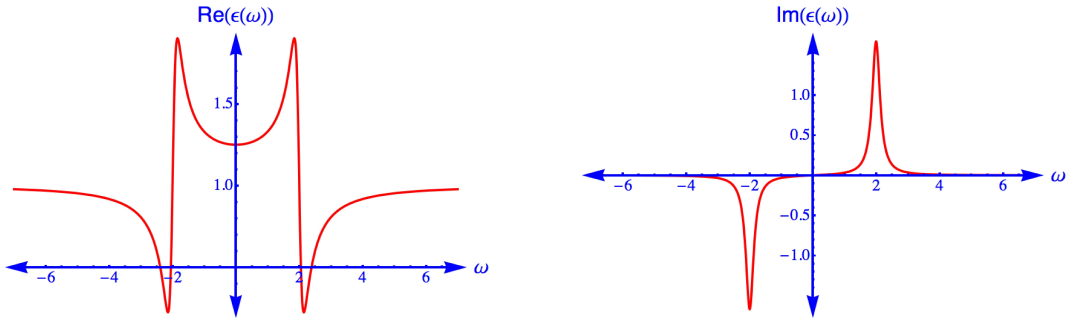

Figure 3.4: Plot of $\mathrm{Re}(\epsilon_r(\omega))$ and $\mathrm{Im}(\epsilon_r(\omega))$ for $\omega_p = 1$, $\omega_0 = 2$, and $\gamma = 0.3$, according to Eq. (3.104). The functional shape of $\mathrm{Re}(\epsilon_r(\omega))$ is consistent with in-phase driving below resonance, with a phase jump by π as one crosses the resonance. The deviation of $\mathrm{Re}(\epsilon_r(\omega))$ from unity at high ω is proportional to $1/\omega^2$.

Restoring prefactors, this can be written as **Relation of Dielectric Constant and Polarizability:**

$$\tilde{\epsilon}(\omega) = \epsilon_0 \left(1 + \frac{N_V}{\epsilon_0}\,\alpha(\omega)\right) = \epsilon_0 \left(1 + \frac{N_V}{\epsilon_0} \sum_n \frac{f_{n0}}{E_{n0}^2 - \mathrm{i}\,\Gamma_n\,\hbar\,\omega - (\hbar\omega)^2}\right). \tag{3.101}$$

If we scale variables according to $E_{n0} \to \hbar\omega_{n0}$ and $\Gamma_n \to \hbar\gamma_n$, then the analogy with a "collection of harmonic oscillators becomes obvious as comparison with Eq. (3.19) shows. Indeed, each term under the sum in Eq. (3.101) has a structure analogous to Eq. (3.19),

$$\widetilde{g}(\omega) = \frac{1}{\omega_0^2 - \mathrm{i}\,\gamma\,\omega - \omega^2}\,. \tag{3.102}$$

Let us briefly discuss an application of the outlined formalism to the famous plasma oscillations, at least within the free-electron gas approximation. First, we observe in Eq. (3.101) that, restricting the sum over n to only a single intermediate state, say $n = 1$, we can replace and define, as appropriate,

$$\frac{N_V}{\epsilon_0}\frac{f_{n0}}{\hbar^2} \to \omega_p^2\,, \qquad \frac{E_{n0}}{\hbar} \to \omega_0\,, \qquad \frac{\Gamma_n}{\hbar} \to \gamma\,. \tag{3.103}$$

Then,

$$\tilde{\epsilon}(\omega) = \epsilon_0 \left(1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - \mathrm{i}\,\omega\,\gamma}\right). \tag{3.104}$$

This is a simple model for a dielectric constant, inspired by a simple harmonic oscillator model (see also Fig. 3.4). The model has the right dimension, as the harmonic oscillator Green function relates the displacement (the position, or "dipole moment") of the driven oscillator to the perturbation, or force, or, electric field.

Let us try to dig a little deeper into this analogy. A free electron gas consists of nearly free electrons, i.e., with a small restorative force, so that the positions of the electrons are described by the formula

$$\ddot{x} + \gamma\,\dot{x} + \omega_0^2\,x = \frac{e}{m_e}\,E_{\mathrm{ext}}(t) \tag{3.105}$$

where x is the (collective) displacement of the (free) electrons in the gas, e is the (physical) electron charge, m_e is the electron mass, and $E_{\mathrm{ext}}(t)$ is the (externally applied) electric field.

In Fourier space, the displacement $\widetilde{x}(\omega)$ is thus given by

$$\widetilde{x}(\omega) = \frac{1}{\omega_0^2 - \omega^2 - \mathrm{i}\,\omega\,\gamma}\,\frac{e}{m_e}\,\widetilde{E}_{\mathrm{ext}}(\omega)\,. \tag{3.106}$$

If N_V is the volume density of plasma electrons, then the volume density of the polarization is given by the formula

$$\widetilde{P}(\omega) = N_V\,e\,\widetilde{x}(\omega) = \frac{1}{\omega_0^2 - \omega^2 - \mathrm{i}\,\omega\,\gamma}\,\left(\frac{N_V\,e^2}{m_e}\right)\,\widetilde{E}_{\mathrm{ext}}(\omega)\,. \tag{3.107}$$

Now,

$$\widetilde{\epsilon}(\omega) = \frac{\epsilon_0\,\widetilde{E}_{\mathrm{ext}}(\omega) + \widetilde{P}(\omega)}{\widetilde{E}_{\mathrm{ext}}(\omega)} = \epsilon_0\,\left[1 + \frac{1}{\omega_0^2 - \omega^2 - \mathrm{i}\,\omega\,\gamma}\,\left(\frac{N_V\,e^2}{\epsilon_0\,m_e}\right)\right] = \epsilon_0\,\left[1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - \mathrm{i}\,\omega\,\gamma}\right]\,, \tag{3.108}$$

where we have identified the plasma frequency ω_p as follows,

$$\omega_p^2 = \frac{N_V\,e^2}{\epsilon_0\,m_e}\,. \tag{3.109}$$

We note the correspondence of Eqs. (3.108) and (3.104). Furthermore, because the electron gas is free, the internal resonance frequency $\omega_0 \ll \omega_p$ is very nearly equal to zero on the scale of the plasma frequency, and we have the the Drude Model of the dielectric constant:

$$\widetilde{\epsilon}(\omega) \approx \epsilon_0\,\left(1 - \frac{\omega_p^2}{\omega^2 + \mathrm{i}\,\omega\,\gamma}\right)\,. \tag{3.110}$$

This formula is canonically known as the Drude model for the dielectric constant of a free electron gas. The so-called plasma model would do away with the term $\mathrm{i}\,\omega\,\gamma$, which would result in an expression which is in conflict with the dispersion relations that have to be fulfilled by the dielectric constant. Basically, the paradigm of these dispersion relations (the so-called Kramers–Kronig relations) is that you cannot have an nontrivial real part in a dielectric constant without also having an imaginary part; dispersion and absorption go hand in hand.

One can also derive the formula for ω_p by different means. Let us consider a bulk material of electrons, with volume density N_V, moving "freely" relative to a jellium of ionized cores, by a collective distance x_c. Let A be the (large) cross-sectional area of the box, and $V = A\,x_c$ its volume. The induced charges of the electrons, "sticking out" at either end of the box, are easily calculated as follows,

$$Q_1 = N_V\,e\,A\,x_c, \qquad Q_2 = -Q_1\,. \tag{3.111}$$

By Gauss's theorem in integrated form, applied to the layer in between the charged structure, we have for the induced electric field $\oint \vec{E}_{\mathrm{ind}} \cdot \mathrm{d}\vec{A} = (\epsilon_0)^{-1}\,\int \mathrm{d}^3 r\,\rho(\vec{r})$, we have

$$E_{\mathrm{ind}}\,A = -\frac{1}{\epsilon_0}\,N_V\,e\,A\,x_c\,, \qquad E_{\mathrm{ind}} = -\frac{1}{\epsilon_0}\,N_V\,e\,x_c\,, \tag{3.112}$$

where the sign follows from a geometric consideration (exercise!). We now express the dielectric constant as follows,

$$\widetilde{\epsilon}(\omega) \approx \epsilon_0\,\frac{\widetilde{E}_{\mathrm{ext}}(\omega) - \widetilde{E}_{\mathrm{ind}}(\omega)}{\widetilde{E}_{\mathrm{ext}}(\omega)}\,. \tag{3.113}$$

Since the electrons in the bulk medium are free, we can approximate

$$m_e\,\frac{\mathrm{d}^2 x_c}{\mathrm{d}t^2} \approx e\,E_{\mathrm{ext}}(t)\,, \qquad -\omega^2\,\frac{m_e}{e}\,\widetilde{x}_c(\omega) \approx \widetilde{E}_{\mathrm{ext}}(\omega)\,, \tag{3.114}$$

where in the latter step we go into Fourier space. Finally,

$$\widetilde{\epsilon}(\omega) \approx \epsilon_0 \, \frac{-\omega^2 \, \dfrac{m_e}{e} \, \widetilde{x}_c(\omega) + \dfrac{1}{\epsilon_0} \, N_V \, e \, \widetilde{x}_c(\omega)}{-\omega^2 \, \dfrac{m_e}{e} \, \widetilde{x}_c(\omega)} = \epsilon_0 \left(1 - \frac{N_V \, e^2}{\epsilon_0 \, m_e} \, \frac{1}{\omega^2} \right) = \epsilon_0 \left(1 - \frac{\omega_p^2}{\omega^2} \right) . \tag{3.115}$$

This "plasma" model ignores the possibility of damping, as given in Eq. (3.110), and, as we later see, does not fulfill the Kramers–Kronig relations, in view of the fact that $\widetilde{\epsilon}(\omega)$ cannot be real everywhere along the real ω-axis. Our model (3.110) thus is physically more consistent than the "plasma" or "bulk" formula (3.115).

Chapter 4

Maxwell Equations and Electrostatics

4.1 Basic Properties of the Maxwell Equations

4.1.1 Integral and Differential Forms of the Maxwell Equations

We recall the Maxwell equations:

$$\text{Gauss's Law:} \qquad \vec{\nabla} \cdot \vec{E}(\vec{r},t) = \frac{1}{\epsilon_0}\,\rho(\vec{r},t)\,, \tag{4.1a}$$

$$\text{Absence of Magnetic Monopoles:} \qquad \vec{\nabla} \cdot \vec{B}(\vec{r},t) = 0\,, \tag{4.1b}$$

$$\text{Faraday's Law:} \qquad \vec{\nabla} \times \vec{E}(\vec{r},t) = -\frac{\partial}{\partial t}\vec{B}(\vec{r},t)\,, \tag{4.1c}$$

$$\text{Ampere–Maxwell Law:} \qquad \vec{\nabla} \times \vec{B}(\vec{r},t) = \mu_0\,\vec{J}(\vec{r},t) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\vec{E}(\vec{r},t)\,. \tag{4.1d}$$

Here, metric (SI) units are employed. We clarify that $\vec{E}$ is the electric field, $\vec{B}$ is the magnetic induction field, μ_0 is the vacuum permeability, ϵ_0 is the vacuum permittivity, ρ is the charge density which measures the electric charge per test volume, and $\vec{J}$ is the current density. Finally, $\vec{\nabla}$ is the gradient operator. The quantity $\vec{\nabla} \cdot \vec{E}$ is the divergence of the electric field, and the quantity $\vec{\nabla} \times \vec{E}$ is the curl of the electric field. Here, $\cdot$ denotes the scalar product and

$$\vec{\nabla} = \hat{\mathrm{e}}_x\,\frac{\partial}{\partial x} + \hat{\mathrm{e}}_y\,\frac{\partial}{\partial y} + \hat{\mathrm{e}}_z\,\frac{\partial}{\partial z} \tag{4.2}$$

is the so-called gradient operator, where $\hat{\mathrm{e}}_x$, $\hat{\mathrm{e}}_y$, and $\hat{\mathrm{e}}_z$ are the unit vectors in the x, y, and z directions. If you are not familiar with any of these quantities, there will be ample opportunity to fill this gap during the following discussion and in further discussions with the course instructor. In writing Eq. (4.1), we have carefully observed that all physical quantities in the Maxwell equations are functions of space and time.

Instead of Eq. (4.1), you may be more familiar with the integral form of the Maxwell equations, which are familiar to you from undergraduate physics. Here, we order them and give them in the form [again in metric

(SI) units]:

$$\textbf{Gauss's Law:} \qquad \int_{\partial V} \vec{E}(\vec{r},t)\cdot \mathrm{d}\vec{A} = \frac{1}{\epsilon_0}\int_V \rho(\vec{r},t)\,\mathrm{d}^3r\,, \tag{4.3a}$$

$$\textbf{Absence of Magnetic Monopoles:} \qquad \int_{\partial V} \vec{B}(\vec{r},t)\cdot \mathrm{d}\vec{A} = 0\,, \tag{4.3b}$$

$$\textbf{Faraday's Law:} \qquad \oint_{\partial A} \vec{E}(\vec{s},t)\cdot \mathrm{d}\vec{s} = -\frac{\partial}{\partial t}\int_A \vec{B}(\vec{r},t)\cdot \mathrm{d}\vec{A}\,, \tag{4.3c}$$

$$\textbf{Ampere–Maxwell Law:} \qquad \oint_{\partial A} \vec{B}(\vec{s},t)\cdot \mathrm{d}\vec{s} = \mu_0\int_A \vec{J}(\vec{r},t)\cdot \mathrm{d}\vec{A} + \frac{1}{c^2}\frac{\partial}{\partial t}\int_A \vec{E}(\vec{r},t)\cdot \mathrm{d}\vec{A}\,. \tag{4.3d}$$

In these equations, V is an arbitrary test volume, and ∂V is its surface, with the surface normal being oriented outward. Also, A is an arbitrary test area, and the "surface" of the test area A is denoted as ∂A. Finally, ∂A is the closed loop that constitutes the outer edge of the area A and therefore is a one-dimensional manifold (line). The sign convention is such that the following three vectors constitute a right-handed system: (i) the line elements $\mathrm{d}\vec{s}$ which are tangent to ∂A (vector 1), (ii) the vector pointing from a line element to the inner region of the area (vector 2), (iii) and the surface normal $\mathrm{d}\vec{A}$ (vector 3). The quantity

$$\int_V \rho(\vec{r},t)\,\mathrm{d}^3r = q_{\mathrm{enclosed}}(t) \tag{4.4}$$

is the enclosed charge in the volume V, still a function of time, and the quantity

$$\int_A \vec{J}(\vec{r},t)\cdot \mathrm{d}\vec{A} = \vec{I}_{\mathrm{inside}}(t) \tag{4.5}$$

is the vector-summed total current penetrating the area A as a function of time. Again, all entities in the Maxwell equations are functions of space and time.

4.1.2 Relation of the Differential to the Integral Form

Transformation of the first and second Maxwell equations. We now investigate how to reconcile the differential form of the Maxwell equations with the integral form, and we start with the first Maxwell equation. Indeed, we start from the integral form Eq. (4.3a) of the first Maxwell equation,

$$\int_{\partial V} \vec{E}(\vec{r},t)\cdot \mathrm{d}\vec{A} = \frac{1}{\epsilon_0}\int_V \rho(\vec{r},t)\,\mathrm{d}^3r\,. \tag{4.6}$$

We now consider a small, but not infinitesimally small test volume $V \to V_\delta$, where V_δ is the cubic volume extending over the intervals $(x, x+\delta x)$, $(y, y+\delta y)$, and $(z, z+\delta z)$, where we consider δx, δy, and δz as small quantities (see also Fig. 4.1). The consideration of small, but not infinitesimally small δx, δy, and δz enables us to perform a Taylor expansion and to discard terms of higher order in the displacements δx, δy, and δz.

Let us consider the yz faces of the test volume V_δ in Fig. 4.1. The outward surface normals are $+\hat{\mathrm{e}}_x$ and $-\hat{\mathrm{e}}_x$. Sampling the electric field in the middle of the test surface, the surface integral can be approximated as

$$I = \left[E_x(x+\delta x, y+\tfrac{1}{2}\delta y, z+\tfrac{1}{2}\delta z, t) - E_x(x, y+\tfrac{1}{2}\delta y, z+\tfrac{1}{2}\delta z, t)\right]\,\delta y\,\delta z\,. \tag{4.7}$$

To first order in δx, we obtain

$$I \approx \frac{\partial}{\partial x} E_x(x, y + \tfrac{1}{2}\delta y, z + \tfrac{1}{2}\delta z, t)\delta x\, \delta y\, \delta z\,. \tag{4.8}$$

If we are interested only in the term proportional to $\delta x\, \delta y\, \delta z$, then we can replace $y + \frac{1}{2}\delta y \to y$, and $z + \frac{1}{2}\delta z \to z$ in the argument of the x component of the electric field. Higher-order terms do not contribute to the order we are interested. In the following, we shall assume that this is possible, as a tacit assumption, and present formulas with the corresponding replacements already implemented.

Thus,

$$I \approx \frac{\partial}{\partial x} E_x(x, y, z, t)\, \delta x\, \delta y\, \delta z \tag{4.9}$$

Indeed, it will turn out that we can choose the sampling point in the direction perpendicular to the surface normal, at an arbitrary point on the "sampled" surface, to leading order in $\delta x\, \delta y\, \delta z$.

With this notion in mind, the left- and right-hand sides of Eq. (4.6) can be written as follows,

$$\begin{aligned}\int_{\partial V_\delta} \vec{E}(\vec{r}, t) \cdot \mathrm{d}\vec{A} \approx\ & \left[E_x(x + \delta x, y + \tfrac{1}{2}\delta y, z + \tfrac{1}{2}\,\delta z, t) - E_x(x, y + \tfrac{1}{2}\delta y, z + \tfrac{1}{2}\,\delta z, t)\right]\, \delta y\, \delta z \\ & + \left[E_y(x + \tfrac{1}{2}\,\delta x, y + \delta y, z + \tfrac{1}{2}\,\delta z, t) - E_y(x + \tfrac{1}{2}\,\delta x, y, z + \tfrac{1}{2}\,\delta z, t)\right]\, \delta x\, \delta z \\ & + \left[E_z(x + \tfrac{1}{2}\,\delta x, y + \tfrac{1}{2}\,\delta y, z + \delta z, t) - E_z(x + \tfrac{1}{2}\,\delta x, y + \tfrac{1}{2}\,\delta y, z, t)\right]\, \delta x\, \delta y\,, \end{aligned} \tag{4.10a}$$

$$\frac{1}{\epsilon_0} \int_{V_\delta} \rho(\vec{r}, t)\, \mathrm{d}^3 r \approx \frac{1}{\epsilon_0} \rho(x + \tfrac{1}{2}\,\delta x, y + \tfrac{1}{2}\,\delta y, z + \tfrac{1}{2}\,\delta z, t)\, \delta x\, \delta y\, \delta z\,. \tag{4.10b}$$

We now approximate as follows,

$$\begin{aligned}&\left[E_x(x + \delta x, y + \tfrac{1}{2}\delta y, z + \tfrac{1}{2}\,\delta z, t) - E_x(x, y + \tfrac{1}{2}\delta y, z + \tfrac{1}{2}\,\delta z, t)\right] \\ &\quad \approx \left[E_x(x + \delta x, y, z, t) - E_x(x, y, z, t)\right] \approx \frac{\partial}{\partial x} E_x(x, y, z, t)\, \delta x\,, \end{aligned} \tag{4.11a}$$

$$\begin{aligned}&\left[E_z(x + \tfrac{1}{2}\,\delta x, y + \tfrac{1}{2}\,\delta y, z + \delta z, t) - E_z(x + \tfrac{1}{2}\,\delta x, y + \tfrac{1}{2}\,\delta y, z, t)\right] \\ &\quad \approx \left[E_y(x, y + \delta y, z, t) - E_y(x, y, z, t)\right] \approx \frac{\partial}{\partial y} E_y(x, y, z, t)\, \delta y\,, \end{aligned} \tag{4.11b}$$

$$\begin{aligned}&\left[E_z(x + \tfrac{1}{2}\,\delta x, y + \tfrac{1}{2}\,\delta y, z + \delta z, t) - E_z(x + \tfrac{1}{2}\,\delta x, y + \tfrac{1}{2}\,\delta y, z, t)\right] \\ &\quad \approx \left[E_z(x, y, z + \delta z, t) - E_z(x, y, z, t)\right] \approx \frac{\partial}{\partial z} E_z(x, y, z, t)\, \delta z\,. \end{aligned} \tag{4.11c}$$

Here, we ignore terms of higher order in the small quantities δx, δy and δz, which would otherwise lead to terms quadratic in the small expansion parameters, such as $\delta x^2\, \delta y\, \delta z$. Proof: Exercise! Analogous approximations are made in Eq. (4.10b).

Inserting Eq. (4.11) into (4.10), we see that the volume $\delta x\, \delta y\, \delta z$ cancels, and so

$$\frac{\partial}{\partial x} E_x(x, y, z, t) + \frac{\partial}{\partial y} E_y(x, y, z, t) + \frac{\partial}{\partial z} E_z(x, y, z, t) = \frac{1}{\epsilon_0} \rho(x, y, z, t)\,. \tag{4.12}$$

For the position vector, we will use the following equivalent representations, according to suitability for a particular purpose,

$$\vec{r} \;=\; x\,\hat{\mathrm{i}} + y\,\hat{\mathrm{j}} + z\,\hat{\mathrm{k}} \;=\; x\,\hat{\mathrm{e}}_x + y\,\hat{\mathrm{e}}_y + z\,\hat{\mathrm{e}}_z \;=\; x_1\,\hat{\mathrm{e}}_1 + x_2\,\hat{\mathrm{e}}_2 + x_3\,\hat{\mathrm{e}}_3 \;=\; \sum_{i=1}^{3} x_i\,\hat{\mathrm{e}}_i\,. \tag{4.13}$$

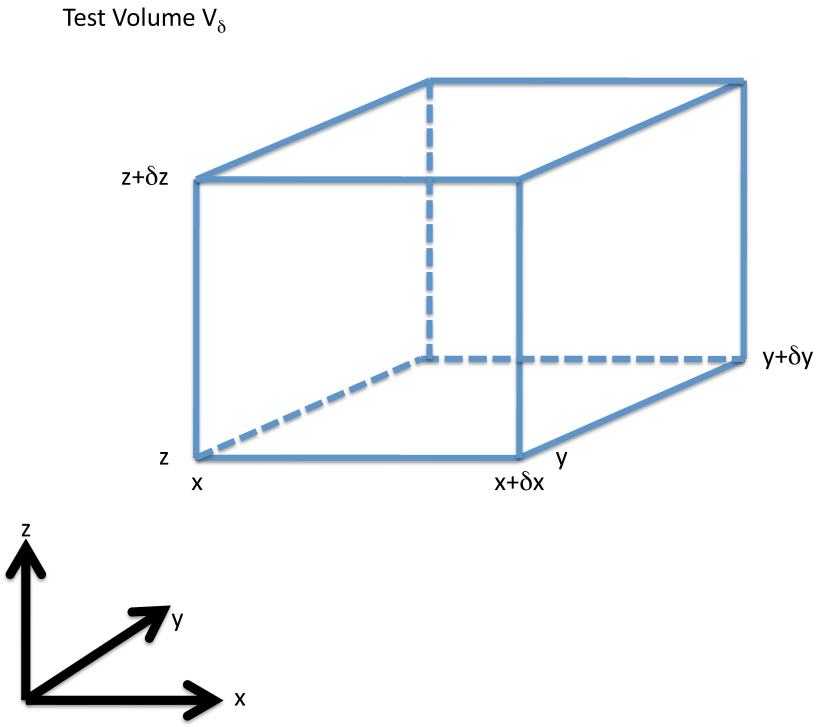

Figure 4.1: Test volume for the transformation of the first and second Maxwell equation from integral to differential form.

The gradient operator is a vector and reads, in Cartesian coordinates,

$$\vec{\nabla} = \hat{\imath}\frac{\partial}{\partial x} + \hat{\jmath}\frac{\partial}{\partial y} + \hat{\mathrm{k}}\frac{\partial}{\partial z} = \hat{\mathrm{e}}_x\frac{\partial}{\partial x} + \hat{\mathrm{e}}_y\frac{\partial}{\partial y} + \hat{\mathrm{e}}_z\frac{\partial}{\partial z} = \hat{\mathrm{e}}_1\frac{\partial}{\partial x_1} + \hat{\mathrm{e}}_2\frac{\partial}{\partial x_2} + \hat{\mathrm{e}}_3\frac{\partial}{\partial x_3} = \sum_{i=1}^{3}\hat{\mathrm{e}}_i\frac{\partial}{\partial x_i}\,, \quad (4.14)$$

where again we use several different representations. We can thus write Eq. (4.12) as

$$\vec{\nabla}\cdot\vec{E}(\vec{r},t) = \frac{1}{\epsilon_0}\,\rho(\vec{r},t)\,, \quad (4.15)$$

which is the differential form of the first Maxwell equation (4.1a). This concludes our discussion of the first Maxwell equation. The transformation of the integral form of the second Maxwell equation (4.3b) into the diffential form (4.1b) is analogous to the above derivation for the first Maxwell equation.

Transformation of the third and fourth Maxwell equations. We now start the discussion of the third Maxwell equation, which involves the curl of the electric field. Its integral form is given in Eq. (4.3c),

$$\oint_{\partial A}\vec{E}(\vec{s},t)\cdot\mathrm{d}\vec{s} = -\frac{\partial}{\partial t}\Phi_B = -\frac{\partial}{\partial t}\int_A\vec{B}(\vec{r},t)\cdot\mathrm{d}\vec{A}\,, \quad (4.16)$$

where Φ_B is the magnetic flux. The closed-loop integral $\oint_{\partial A}\vec{E}(\vec{s},t)\cdot\mathrm{d}\vec{s}$ involves the electric field $\vec{E}(\vec{s},t)$ at the position $\vec{s}$ on the line integral. We assume that the test area A_δ is oriented in the xy plane so that its surface normal is oriented along the positive z axis. The test area extends over the interval $(x, x+\delta x)$ in the x-direction and over the interval $(y, y+\delta y)$ in the y-direction, at an arbitrary z coordinate (see also Fig. 4.2).

We encircle the line integral about the infinitesimal test area $A \to \partial A_\delta$ in the counterclockwise direction and pick up the contributions. We can then approximate for the two sides of Eq. (4.16),

$$\oint_{\partial A_\delta} \vec{E}(\vec{s},t)\cdot \mathrm{d}\vec{s} \approx E_x(x+\tfrac{1}{2}\,\delta x, y, z, t)\;\delta x + E_y(x+\delta x, y+\tfrac{1}{2}\,\delta y, z, t)\;\delta y$$
$$- E_x(x+\tfrac{1}{2}\,\delta x, y+\delta y, z)\;\delta x - E_y(x, y+\tfrac{1}{2}\,\delta y, z, t)\;\delta y\,, \tag{4.17}$$

$$-\frac{\partial}{\partial t}\int_{A_\delta} \vec{B}(\vec{r},t)\cdot \mathrm{d}\vec{A} \approx\; -\frac{\partial}{\partial t} B_z(x+\tfrac{1}{2}\delta x, y+\tfrac{1}{2}\delta y, z, t)\;\delta x\,\delta y\,. \tag{4.18}$$

(We have pedantically used the half-way approximations on the sides of the rectangle that are not being varied.) By a Taylor expansion δx, δy, and δz, we obtain

$$-\frac{\partial}{\partial y} E_x(x,y,z,t)\;\delta x\,\delta y + \frac{\partial}{\partial x} E_y(x,y,z,t)\;\delta x\,\delta y \approx -\frac{\partial}{\partial t} B_z(x,y,z,t)\;\delta x\,\delta y\,. \tag{4.19}$$

Cancelling the test area $\delta x\,\delta y$, we obtain from Eq. (4.16),

$$\frac{\partial}{\partial x} E_y - \frac{\partial}{\partial y} E_x = \left(\vec{\nabla}\times\vec{E}\right)_z = -\frac{\partial}{\partial t} B_z\,, \tag{4.20}$$

where we suppress the space-time arguments of the fields. We have obtained the z-component of Eq. (4.16), as we identify $\frac{\partial}{\partial x}E_y - \frac{\partial}{\partial y}E_x$ as the z component of the curl of the electric field. In general, the curl of a vector field is defined as

$$\vec{\nabla}\times\vec{E} = \det\begin{pmatrix} \hat{\mathrm{e}}_x & \hat{\mathrm{e}}_y & \hat{\mathrm{e}}_z \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ E_x & E_y & E_z \end{pmatrix}. \tag{4.21}$$

With reference to Eq. (4.13) and (4.14), its components are given as

$$(\vec{\nabla}\times\vec{E})_i = \sum_{j=1}^{3}\sum_{k=1}^{3} \epsilon_{ijk}\frac{\partial}{\partial x_j}E_k\,, \qquad i=1,\ldots,3; \quad j=1,\ldots,3; \quad k=1,\ldots,3\,. \tag{4.22}$$

where we identify $E_1 = E_x$ as the x-component, $E_2 = E_y$ as the y-component, and $E_3 = E_z$ as the z-component. Here, ϵ_{ijk} is the totally antisymmetric tensor, i.e., $\epsilon_{123} = 1$, and ϵ_{ijk} is equal to the sign of the permutation that transforms the triple $(1,2,3)$ into (i,j,k). If an even number of exchanges of number is required in order to transform $(1,2,3)$ into (i,j,k), then the sign of the permutation is 1, otherwise it is -1. So, $\epsilon_{231} = 1$, but $\epsilon_{213} = -1$. If two of the indices are equal, such as in $\epsilon_{122} = 0$, the result is zero. The verification of Eq. (4.22) is left as an exercise. We can also write

$$\vec{\nabla}\times\vec{E} = \sum_{i=1}^{3}\sum_{j=1}^{3}\sum_{k=1}^{3} \hat{\mathrm{e}}_i\,\epsilon_{ijk}\frac{\partial}{\partial x_j}E_k\,. \tag{4.23}$$

In the above derivation leading to (4.20), we have assumed the test area ∂A to be oriented along the positive z axis. If we change the orientation of the test area A_δ, then we recover the x and y components of the equation

$$\vec{\nabla}\times\vec{E} = -\frac{\partial}{\partial t}\vec{B}\,, \tag{4.24}$$

where we suppress the space-time arguments of the electric and magnetic fields. This concludes our discussion of the third Maxwell equation. The transformation of the fourth Maxwell equation from integral to differential form is analogous.

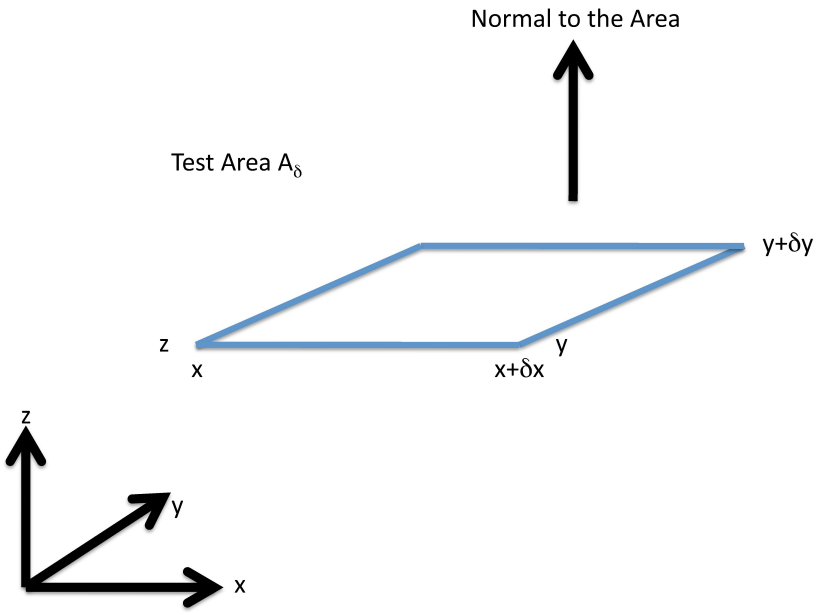

Figure 4.2: Test area for the transformation of the third and fourth Maxwell equation from integral to differential form.

Continuity Equation. One of the most paradigmatic applications of the formalism outlined above involves the so-called continuity equation. The continuity equation is a simple statement that says that the charge leaving a test volume V through currents can be obtained in two alternative ways: (i) as the currrent density $\vec{j}$ summed over the surface area of the test volume ∂V, and (ii) as the time derivative of the charge density, summed/integrated over the test volume V. This means that

$$\int_{\partial V} \vec{J}(\vec{r},t)\cdot \mathrm{d}\vec{A} = -\frac{\partial}{\partial t}\int_V \rho(\vec{r},t)\,\mathrm{d}^3 r\,, \tag{4.25}$$

which is the integral form of the continuity equation. Using the same test volume as before, we obtain [see Eq. (4.11)]

$$\begin{aligned}
&\left[J_x(x+\delta x, y+\tfrac{1}{2}\delta y, z+\tfrac{1}{2}\delta z, t) - J_x(x, y+\tfrac{1}{2}\delta y, z+\tfrac{1}{2}\delta z, t)\right]\,\delta y\,\delta z + \\
&\left[J_y(x+\tfrac{1}{2}\delta x, y+\delta y, z+\tfrac{1}{2}\delta z, t) - J_y(x+\tfrac{1}{2}\delta x, y, z+\tfrac{1}{2}\delta z, t)\right]\,\delta x\,\delta z + \\
&\left[J_z(x+\tfrac{1}{2}\delta x, y+\tfrac{1}{2}\delta y, z+\delta z, t) - J_z(x+\tfrac{1}{2}\delta x, y+\tfrac{1}{2}\delta y, z, t)\right]\,\delta x\,\delta y \\
&\qquad = -\frac{\partial}{\partial t}\rho(x+\tfrac{1}{2}\delta x, y+\tfrac{1}{2}\delta y, z+\tfrac{1}{2}\delta z, t)\,\delta x\,\delta y\,\delta z\,.
\end{aligned} \tag{4.26}$$

Expanding into a Taylor series and cancelling the test volume $\delta x\,\delta y\,\delta z$, we obtain

$$\frac{\partial}{\partial x}J_x(x,y,z,t) + \frac{\partial}{\partial y}J_y(x,y,z,t) + \frac{\partial}{\partial z}J_z(x,y,z,t) = -\frac{\partial}{\partial t}\rho(x,y,z,t)\,. \tag{4.27}$$

Then, the differential form of the continuity equation is obtained,

$$\vec{\nabla}\cdot\vec{J} + \frac{\partial}{\partial t}\rho = 0\,, \tag{4.28}$$

where again we suppress the space-time arguments of the current and charge density.

4.2 Maxwell Equations in Vacuum

4.2.1 Electrostatics and Coulomb's law

Coulomb's Law. The Maxwell equations govern the temporal and spatial variations of electromagnetic fields and their coupling to the sources ρ and $\vec{J}$. They have to be complemented by the continuity equation and by the Lorentz force law in order to form a self-consistent set of equations that also describes the back-reaction of the fields on the sources. However, historically, the electric phenomena were discovered first in terms of the forces (not fields) exerted on test objects. Indeed, the results of the numerous investigations of electromagnetic phenomena carried out during the 18^{th} and 19^{th} centuries led to the development of a set of equations which describe these phenomena. Indeed, in the previous section, we have first considered the Maxwell equations (4.1) as a "God-given" set of equations and convinced ourselves that they are equivalent to the integral forms of the equations which may still be familiar to you from PHYSICS 24. Now, we follow the historic route and first study the forces on test objects due to electromagnetic interactions. After that, we relate these forces to the abstract concept of fields, and then, we investigate how the fields are related to their sources (charge and current distributions). From these investigations, we then deduce a set of equations which are equivalent to the one already given in Eq. (4.1). We go "the other way" and take "Route 66" instead of the "Interstate."

The first observational law established in electromagnetic theory is Coulomb's law, which provided the description of the force, $\vec{F}_{12} = \vec{F}_{1\leftarrow 2}$, on a stationary point particle at $\vec{r}_1$ of electric charge q_1 due to a stationary point particle with charge q_2 located at $\vec{r}_2$. Note that the quantities $\vec{r}_1$ and $\vec{r}_2$ are vectors.

We shall see that it is possible to complement mechanical units by electromagnetic units in various ways, and to form relations among mechanical and electromagnetic units if the force laws are written in specific forms. Thus, in the following statement of Coulomb's law, the parameter $\frac{1}{4\pi\epsilon_0}$ is a constant determined by the system of units. The electrostatic force acting on body 1 due to the presence of body 2 reads

$$\vec{F}_{12} \equiv \vec{F}_{1\leftarrow 2} = \frac{1}{4\pi\epsilon_0}\frac{q_1\,q_2}{|\vec{r}_1-\vec{r}_2|^3}\,(\vec{r}_1-\vec{r}_2) = \frac{1}{4\pi\epsilon_0}\frac{q_1\,q_2}{r_{12}^2}\,\hat{r}_{12}\,, \qquad \vec{r}_{12} = \vec{r}_1-\vec{r}_2\,, \qquad \hat{r}_{12} = \frac{\vec{r}_{12}}{r_{12}}\,, \tag{4.29}$$

where $r_{12} = |\vec{r}_{12}|$ is the distance of body number 1 to body number 2. Note that the vector $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$ points from body 2 to body 1, as it should (see also Fig. 4.3). We here use the SI mksA international system of units. The use of the Ampere as the fundamental unit of current fixes the Coulomb as the fundamental unit of charge, because it is obtained as the product of the fundamental unit of current (Ampere) and the fundamental unit of time, which is the second. First of all, in order to practice the unit conversion in the SI mksA system, we show the relation

$$10^{-7}\,c^2\,\frac{\mathrm{V\,s}}{\mathrm{A\,m}} \approx 9\cdot 10^9\,\mathrm{N}\,\frac{\mathrm{m}^2}{\mathrm{C}^2}\,, \tag{4.30}$$

where the numerical values on the right-hand side is approximate. The unit conversion is as follows,

$$10^{-7}\,c^2\,\frac{\mathrm{V\,s}}{\mathrm{A\,m}} \approx 10^{-7}\,(3\cdot 10^8\mathrm{m/s})^2\,\frac{\mathrm{V\,s}}{\mathrm{A\,m}} = 9\cdot 10^9\,\frac{\mathrm{m}^2}{\mathrm{s}^2}\,\frac{\mathrm{N\,m\,s}^2}{\mathrm{C}^2\,\mathrm{m}} = 9\cdot 10^9\,\frac{\mathrm{m}^2}{\mathrm{s}^2}\,\frac{\mathrm{N\,m\,s}^2}{\mathrm{C}^2\,\mathrm{m}} = 9\cdot 10^9\,\mathrm{N}\,\frac{\mathrm{m}^2}{\mathrm{C}^2}\,. \tag{4.31}$$

It is perhaps surprising to remember that the concept of an (electric) field was quite novel when it was introduced by Maxwell. First and foremost, a field is a physical, time- and position-dependent quantity which does not need to be detected in order to exist. A force, by contrast, acts on a body; if it does not act, then it does not exist. A field only acts on a body when a suitable test particle is present. Secondly, a field may be scalar-valued (it may be a dimensionless number or a dimensionful physical quantity such as a potential, whose value depends on space and time), or a vector whose value is space- and time-dependent.

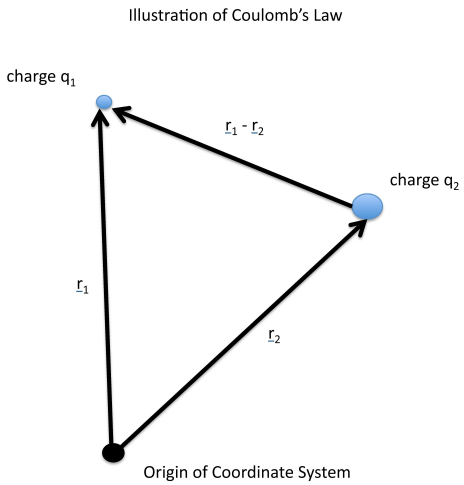

Figure 4.3: Illustration of Coulomb's Law. Note that formula (4.29) gives both the right magnitude as well as the right direction of the force exerted by charge 1 onto charge 2.

In the case of a static electric field,

$$\vec{E} = \vec{E}\left(\vec{r}_1\right), \tag{4.32}$$

the field is vector-valued and the values of all three components of the vector depend on space. Let us start with a time-independent field), generated by electrically charged point particles

$$\vec{E}\left(\vec{r}_1\right) = \frac{1}{4\pi\epsilon_0} \frac{q_2}{|\vec{r}_1 - \vec{r}_2|^3} \left(\vec{r}_1 - \vec{r}_2\right) . \tag{4.33}$$

This observation allowed a local force law on point charges to be developed,

$$\vec{F}_{12} = q_1 \vec{E}_{(2)}\left(\vec{r}_1\right) . \tag{4.34}$$

Here, q_1 acts as the test particle for the detection of the field at its own location, i.e., $\vec{r}_1$. The field itself is generated by the charge q_2 located at point $\vec{r}_2$ and is present even if we do not observe it by the presence of the probe charge q_1 (concept of a **field)**. The electric force (4.34) also holds when the electric field is time-dependent,

$$\boxed{\textbf{Electric Force:}} \qquad \vec{F} = q\,\vec{E}\left(\vec{r}, t\right) , \tag{4.35}$$

where we denote the test charge as q and the time-dependent electric field as $\vec{E}\left(\vec{r}, t\right)$.

4.2.2 Superposition Principle and Continuum Limit

The superposition principle holds for the electric field and if $\{q_i,\, i = 1, ..., N\}$ are the charges of N point particles located at the points $\{\vec{r}_i,\, i = 1, \ldots, N\}$. The charges q_i are the sources of the electric field, which are located at points $\vec{r}_i$. At a detection point $\vec{r}$, the field is given as the sum of the fields generated by the individual sources,

$$\vec{E}\left(\vec{r}\right) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^{N} \frac{q_i}{\left|\vec{r} - \vec{r}_i\right|^3} \left(\vec{r} - \vec{r}_i\right) \tag{4.36}$$

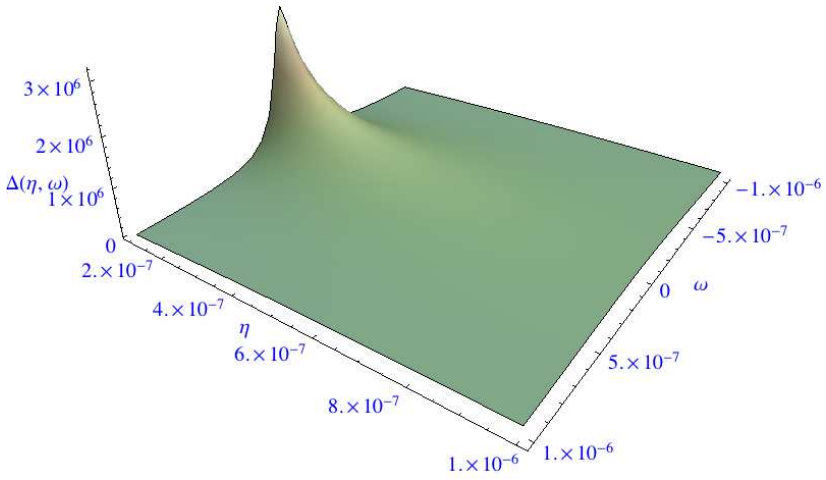

Figure 4.4: Graphical illustration of the Dirac δ function.

If there are many densely distributed charges (so that macroscopically they can be described by a continuous charge density),

$$\frac{\mathrm{d}q(\vec{r})}{\mathrm{d}V} = \rho\left(\vec{r}\right) , \tag{4.37}$$

then the electric field is given as the generalization of Eq. (4.36) to integral form,

$$\vec{E}\left(\vec{r}\right) = \frac{1}{4\pi\epsilon_0} \int_V \left(\frac{\vec{r} - \vec{r}'}{\left|\vec{r} - \vec{r}'\right|^3} \right) \frac{\mathrm{d}q(\vec{r})}{\mathrm{d}V} \, dV' = \frac{1}{4\pi\epsilon_0} \int_V \left(\frac{\vec{r} - \vec{r}'}{\left|\vec{r} - \vec{r}'\right|^3} \right) \rho\left(\vec{r}'\right) \mathrm{d}^3 r' \, . \tag{4.38}$$

Here, V is the entire volume in which the charge density $\rho(\vec{r})$ is nonzero, i.e. $\rho(\vec{r}) = 0$ if $\vec{r}$ is outside V.

In order to go back from Eq. (4.38) to Eq. (4.36), one needs the Dirac δ function in order to be able to formulate a charge density describing point charges. This function (or, more precisely, this distribution) is useful in a more general context, in order to relate electric fields to their sources. A possible representation of the Dirac δ function (see Sec. 2.2.1) is

$$\delta(\omega) = \Delta(\eta, \omega) = \frac{1}{\pi} \frac{\eta}{\omega^2 + \eta^2} \, , \qquad \eta \to 0^+ \, , \tag{4.39}$$

where the limit is approached *nonuniformly*. It has the properties

$$\int_{-\infty}^{\infty} \mathrm{d}\omega \, \Delta(\eta, \omega) = 1 \, , \tag{4.40a}$$

$$\lim_{\eta \to 0^+} \Delta(\eta, \omega) = 0 \quad (\text{for } \omega \neq 0), \tag{4.40b}$$

$$\lim_{\eta \to 0^+} \Delta(\eta, \omega) = \infty \quad (\text{for } \omega = 0), \tag{4.40c}$$

$$\int_{-\infty}^{\infty} \mathrm{d}\omega \left[\lim_{\eta \to 0^+} \Delta(\eta, \omega) \right] f(\omega) = 0 \, , \qquad \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega \, \Delta(\eta, \omega) \, f(\omega) = f(0) \, . \tag{4.40d}$$

The last two properties illustrate that one cannot take the limit $\eta \to 0$ too early (keyword: non-uniform convergence). A graphical illustration can be found in Fig. 4.4. In the limit $\eta \to 0^+$, then, $\Delta(\eta, \omega) \to \delta(\omega)$. Alternatively, and axiomatically, one can define the (one-dimensional) Dirac delta function by the condition

$$\int_a^b f\left(x'\right) \, \delta\left(x - x'\right) \, \mathrm{d}x' = f\left(x\right) \qquad \text{if} \qquad a < x < b \, , \tag{4.41}$$

and

$$\int_a^b f(x')\,\delta(x-x')\,\mathrm{d}x' = 0 \qquad \text{if} \qquad x < a \qquad \text{or} \qquad x > b\,. \tag{4.42}$$

If $x = a$ or $x = b$, the integral is not well defined, but a common definition is

$$\int_a^b f(x')\,\delta(x-x')\,\mathrm{d}x' = \tfrac{1}{2}\,f(x) \qquad \text{for} \qquad x = a \qquad \text{or} \qquad x = b\,. \tag{4.43}$$

This definition is inspired by the fact that any representation of the Dirac-δ function which is symmetric about the centre yields the result (4.43). If the argument of a Diract delta function is a function of x,

$$\delta(f(x)) = \sum_{i=1}^{n} \left(\left| \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{x=x_i} \right| \right)^{-1} \delta(x - x_i)\ , \tag{4.44}$$

where the x_i $(i = 1, \ldots, n)$ with $g(x_i) = 0$ denote simple zeros of $g(x)$. The three-dimensional delta function is equal to the product of three one-dimensional Dirac delta functions,

$$\delta^{(3)}(\vec{r} - \vec{r}') = \delta(x - x')\,\delta(y - y')\,\delta(z - z')\,. \tag{4.45}$$

Thus,

$$\int_V \mathrm{d}x'\mathrm{d}y'\mathrm{d}z'\ f(\vec{r}')\ \delta^{(3)}(\vec{r} - \vec{r}') = f(\vec{r}) \qquad \text{if } \vec{r} \text{ is interior to the volume } V \text{ and } 0 \text{ otherwise.} \tag{4.46}$$

For multiple integrals such as $\int_V$ (over the three-dimensional volume V), we here follow the convention that the integration domain is being indicated by a subscript to the integral sign; the integration domain then automatically defines the dimensionality of the integral.

Starting from

$$\vec{E}(\vec{r}) = \frac{1}{4\pi\epsilon_0} \int_V \left(\frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|^3} \right) \rho(\vec{r}')\,\mathrm{d}^3 r'\,. \tag{4.47}$$

and setting

$$\rho(\vec{r}') = \sum_{i=1}^{N} q_i\,\delta^{(3)}(\vec{r}' - \vec{r}_i) \tag{4.48}$$

in order to describe N point charges q_i located at positions $\vec{r}_i$ with $i = 1, \ldots, N$, we obtain

$$\vec{E}(\vec{r}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^{N} q_i\,\frac{\vec{r} - \vec{r}_i}{|\vec{r} - \vec{r}_i|^3} \tag{4.49}$$

with the help of Eq. (4.46). This completes the way back from Eq. (4.38) to Eq. (4.36), with the help of the Dirac δ function.

4.2.3 From the Coulomb Force Law to Gauss's Law

Formula (4.38) allows us to calculate the static electric field for continuous charge distributions. Using the Dirac δ function, we may rewrite this formula in terms of Gauss's law. We start from

$$\vec{E}(\vec{r}) = \frac{1}{4\pi\epsilon_0} \int_V \left(\frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|^3} \right) \rho(\vec{r}')\,\mathrm{d}^3 r'\,. \tag{4.50}$$

We can write the integrand in terms of the gradient operator, $\vec{\nabla}$, with respect to the $\vec{r}$ coordinate vector:

$$-\vec{\nabla}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)=\frac{1}{|\vec{r}-\vec{r}'|^2}\,\vec{\nabla}\,|\vec{r}-\vec{r}'|=\frac{1}{|\vec{r}-\vec{r}'|^2}\cdot\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|} \tag{4.51}$$

where we take notice of the fact that

$$\vec{\nabla}\,|\vec{r}-\vec{r}'|=\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|} \tag{4.52}$$

is a unit vector along the $\vec{r}-\vec{r}'$ direction. The electric field (4.50) can thus be written as

$$\vec{E}\,(\vec{r})=\frac{1}{4\pi\epsilon_0}\int_V\left(-\vec{\nabla}\frac{1}{|\vec{r}-\vec{r}'|}\right)\rho\,(\vec{r}')\,\mathrm{d}^3r'\,. \tag{4.53}$$

If one takes $\vec{\nabla}\cdot\vec{E}\,(\vec{r})$,

$$\vec{\nabla}\cdot\vec{E}\,(\vec{r})=\frac{1}{4\pi\epsilon_0}\int_V\left(-\vec{\nabla}\cdot\vec{\nabla}\frac{1}{|\vec{r}-\vec{r}'|}\right)\rho\,(\vec{r}')\,\mathrm{d}^3r'\,, \tag{4.54}$$

and uses the following identity, shown below,

$$\vec{\nabla}\cdot\vec{\nabla}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)=\vec{\nabla}^2\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)=-4\pi\,\delta^{(3)}(\vec{r}-\vec{r}')\,, \tag{4.55}$$

then Eq. (4.54) becomes

Gauss's Law (electrostatics): $$\vec{\nabla}\cdot\vec{E}\,(\vec{r})=\frac{1}{\epsilon_0}\,\rho\,(\vec{r})\,. \tag{4.56}$$

It remains to show the identity (4.55),

Dirac δ function: $$\vec{\nabla}^2\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)=-4\pi\,\delta^{(3)}(\vec{r}-\vec{r}')\,. \tag{4.57}$$

Even if this identity was already discussed in Sec. 3.3.2, we present a discussion adapted to the three-dimensional case. We start from the left-hand side and apply the divergence theorem,

$$\int_V\mathrm{d}^3r'\,\vec{\nabla}^2\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)=\int_{\partial V}\vec{\nabla}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\cdot\mathrm{d}\vec{A}=-\int_{\partial V}\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|^3}\cdot\mathrm{d}\vec{A}\,. \tag{4.58}$$

We now choose as V an infinitesimally small sphere about the point $\vec{r}'$, still containing $\vec{r}'$, and centered at $\vec{r}'$. Let its radius be R. Then, $(\vec{r}-\vec{r}')/\,|\vec{r}-\vec{r}'|^3$ is an outward normal pointing to the outside of the sphere, of magnitude $1/R^2$. We evaluate the integral as follows,

$$-\int_{\partial V}\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|^3}\cdot\mathrm{d}\vec{A}=-\frac{1}{R^2}\,4\pi R^2=-4\pi\,. \tag{4.59}$$

As a result, we have shown that

$$\int_V\mathrm{d}^3r'\,\vec{\nabla}^2\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)=-4\pi \tag{4.60}$$

for any sphere about $\vec{r}'$. This can only be fulfilled if the identity (4.57) holds. Once more, in a slightly different fashion, we consider the application of Gauss's theorem,

$$\int_{\partial V}\vec{V}(\vec{r})\cdot\mathrm{d}\vec{A}=\int_V\vec{\nabla}\cdot\vec{V}(\vec{r})\,\mathrm{d}V\,, \tag{4.61}$$

to a sphere S_ϵ of radius R_ϵ with surface ∂S_ϵ,

$$-4\pi = -\frac{4\pi}{R_\epsilon^2}\, R_\epsilon^2 = \vec{\nabla} \int_{\partial S_\epsilon} \frac{1}{|\vec{r}-\vec{r}'|}\, \mathrm{d}\vec{A} = \int_{S_\epsilon} \left(\vec{\nabla}^2 \frac{1}{|\vec{r}-\vec{r}'|} \right) \mathrm{d}^3 r' \,. \tag{4.62}$$

As we let $R_\epsilon \to 0$, and consider the fact that

$$\vec{\nabla}^2 \frac{1}{|\vec{r}-\vec{r}'|} = 0\,, \qquad \vec{r} \neq \vec{r}'\,, \tag{4.63}$$

which has been shown in the exercises, we see that the only distribution/function of $\vec{r}$ that could fulfill this relation is indeed given by the identity (4.57).

We can immediately apply this formalism to the electrostatics of a point charge. The charge distribution $\rho = \rho_{\text{point}}\,(\vec{r})$ at the point $\vec{r}$ due to a point particle with charge q_2 at the point $\vec{r}_2$ reads

$$\rho_{\text{point}}\,(\vec{r},\ \vec{r}_2) = q\ \delta^{(3)}\,(\vec{r}-\vec{r}_2)\ . \tag{4.64}$$

Here, the three-dimensional Dirac delta function is given by [see also Eq. (4.45)]

$$\delta^{(3)}(\vec{r}-\vec{r}_2) = \delta(x-x_2)\,\delta(y-y_2)\,\delta(z-z_2)\,. \tag{4.65}$$

A solution to the partial differential equation

$$\vec{\nabla}\cdot\vec{E}_{\text{point}}\,(\vec{r}) = \frac{1}{\epsilon_0}\rho_{\text{point}}\,(\vec{r})\ , \qquad \vec{E}_{\text{point}}\,(\vec{r},\vec{r}_2) = \frac{1}{4\pi\epsilon_0}\,\frac{q_2}{|\vec{r}-\vec{r}_2|^3}\,(\vec{r}-\vec{r}_2)\ , \tag{4.66}$$

is the electric field due to a charged point particle located at $\vec{r}_2$. We verify that

$$\begin{aligned}\vec{\nabla}\cdot\vec{E}_{\text{point}}\,(\vec{r}) &= \frac{1}{4\pi\epsilon_0}\,q_2\,\vec{\nabla}\cdot\left(-\vec{\nabla}\frac{1}{|\vec{r}-\vec{r}_2|}\right) = -\frac{1}{4\pi\epsilon_0}\,q_2\,\vec{\nabla}^2\frac{1}{|\vec{r}-\vec{r}_2|} \\ &= \frac{1}{\epsilon_0}\,q_2\,\delta^{(3)}(\vec{r}-\vec{r}_2) = \frac{1}{\epsilon_0}\,\rho_{\text{point}}\,(\vec{r},\vec{r}_2)\ .\end{aligned} \tag{4.67}$$

4.2.4 Electrostatic Potential and Curl of the Static Field

Due to Gauss's law, the divergence of the static electric field, $\vec{\nabla}\cdot\vec{E}\,(\vec{r})$, is nonvanishing only in those spatial regions where the electrostatic charge density is also nonvanishing. However, the curl of a vector field is as important to its description as is the divergence. Indeed, for the curl of the static electric field, one can derive, using Eq. (4.51),

$$\vec{\nabla}\times\vec{E}\,(\vec{r}) = \vec{\nabla}\times\frac{1}{4\pi\epsilon_0}\int_V \left(-\vec{\nabla}\frac{1}{|\vec{r}-\vec{r}'|}\right)\rho\,(\vec{r}')\,\mathrm{d}^3r' = 0 = -\frac{1}{4\pi\epsilon_0}\int_V \left(\left(\vec{\nabla}\times\vec{\nabla}\right)\frac{1}{|\vec{r}-\vec{r}'|}\right)\rho\,(\vec{r}')\,\mathrm{d}^3r' = \vec{0} \tag{4.68}$$

because in general,

$$\vec{\nabla}\times\vec{\nabla}f(\vec{r}) = 0$$

and so, in particular,

$$\vec{\nabla}\times\vec{\nabla}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right) = 0\,. \tag{4.69}$$

The equations

Electric Field in Electrostatics: $$\vec{\nabla}\cdot\vec{E}\,(\vec{r}) = \frac{1}{\epsilon_0}\rho\,(\vec{r})\ , \qquad \vec{\nabla}\times\vec{E}\,(\vec{r}) = 0\,, \tag{4.70}$$

thus define the behavior of $\vec{E}\,(\vec{r})$ in electrostatics. To determine $\vec{E}\,(\vec{r})$ uniquely, one must also have boundary conditions on $\vec{E}\,(\vec{r})$. Indeed, for a vector field that fulfills $\vec{\nabla}\cdot\vec{E}\,(\vec{r}) = 4\pi\frac{1}{4\pi\epsilon_0}\rho\,(\vec{r})$ and $\vec{\nabla}\times\vec{E}\,(\vec{r}) = 0$, one can trace the physical origin of the vector field to the concept of a potential, which we discuss in the following.

Sometimes it is easier to deal with scalar functions, which leads us directly to the concept of the electrostatic potential. From $\vec{\nabla}\times\vec{E}\,(\vec{r}) = 0$ (see also the discussion below), one can assume that

$$\vec{E}\,(\vec{r}) = -\vec{\nabla}\Phi\,(\vec{r})\;. \tag{4.71}$$

From the integral form for $\vec{E}\,(\vec{r})$ given in Eq. (4.53), we can directly read off the following integral representation

$$\Phi\,(\vec{r}) = \frac{1}{4\pi\epsilon_0}\int_V \frac{\rho\,(\vec{r}')}{|\vec{r}-\vec{r}'|}\,\mathrm{d}^3r' + \Phi_0\,, \qquad \vec{\nabla}^2\,\Phi(\vec{r}) = -\frac{1}{\epsilon_0}\,\rho(\vec{r})\,, \qquad \vec{\nabla}^2\,\Phi_0(\vec{r}) = 0\,. \tag{4.72}$$

One might think that, at this point, the entire field of electrostatics has been trivialized in the sense that a general solution for the electric field as a function of the charge density has been written down. This is not the case, however. Namely, one overlooks two aspects. The first is that the solution of any differential equation not only depends on the source term, but also on the boundary conditions. Even, highly nontrivial solutions of the Laplace equation $\vec{\nabla}^2\,\Phi(\vec{r}) = 0$ exist, depending on the boundary conditions. We will study these in the following. To illustrate this aspect further, one might observe that the Green function in three dimensions, given in Eq. (3.68),

$$g(\vec{r}-\vec{r}') = -\frac{1}{4\pi|\vec{r}-\vec{r}'|}\,, \qquad \vec{\nabla}^2 g(\vec{r}-\vec{r}') = \delta^{(3)}(\vec{r}-\vec{r}')\,, \tag{4.73}$$

constitutes a Green function of the Poisson equation which fulfills vanishing boundary conditions at infinity. A potential calculated according to Eq. (4.72) may not fulfill the given boundary conditions in a particular experimental configuration. The second aspect which illustrates that we should not stop our investigations is that, even in cases where the charge distribution $\rho = \rho(\vec{r}')$ is given, the evaluation of the three-dimensional integral in Eq. (4.72) can be problematic and may only be feasible in terms of a multipole decomposition, which we will discuss in the following.

One can relate the potential $\Phi\,(\vec{r})$ to the work done in moving a charged particle under the influence of a force field. Indeed, the force acting on a test particle with charge q is

$$\boxed{\textbf{Electric Force Law:}} \qquad \vec{F}\,(\vec{r}) = q\,\vec{E}\,(\vec{r})\;. \tag{4.74}$$

If we wish to move a test particle through the electrostatic field, then we have to compensate the electrostatic force, i.e. we have to exert a force $-\vec{F}\,(\vec{r})$ onto the particle. The electrostatic potential, $\Phi\,(\vec{r})$, is the electrostatic potential energy (of a unit test charge) in the electric field, $\vec{E}\,(\vec{r})$, and is related to the work done by an external force in moving a charge, q, from $\vec{r}_0$ to $\vec{r}$:

$$\begin{aligned} W &= \int_{\vec{r}_0}^{\vec{r}} \Big(-\vec{F}(\vec{s}')\Big)\cdot\mathrm{d}\vec{s}' = -\int_{\vec{r}_0}^{\vec{r}} q\,\vec{E}\,(\vec{s}')\cdot\mathrm{d}\vec{s}' = \int_{\vec{r}_0}^{\vec{r}} q\,\vec{\nabla}\Phi\,(\vec{s}')\cdot\mathrm{d}\vec{s}' \\ &= \int_{\vec{r}_0}^{\vec{r}} q\,[\mathrm{d}\vec{s}'\cdot\vec{\nabla}\,\Phi\,(\vec{s}')] = \int_{\vec{r}_o}^{\vec{r}} q[\mathrm{d}\Phi\,(\vec{s})] = q[\Phi\,(\vec{r}) - \Phi\,(\vec{r}_0)]\,. \end{aligned} \tag{4.75}$$

Note that in $-\vec{F}(r')\cdot d\vec{r}'$, the negative sign denotes work done *against* the electric field, not work done *by* the field. Here, we have used the following useful relation, which you should know and be able to use:

$$\mathrm{d}\vec{r}\cdot\vec{\nabla}f\,(\vec{r}) = \mathrm{d}f \qquad \text{(a perfect differential)}\,. \tag{4.76}$$

We supplement the discussion by a few remarks on the unique decomposition of a vector field into longitudinal and perpendicular components. Let us consider the time-independent situation. In general, any vector field that is a function of position, $\vec{V}(\vec{r})$, can be written as the sum of two vector fields,

$$\vec{V}(\vec{r}) = \vec{V}_{\parallel}(\vec{r}) + \vec{V}_{\perp}(\vec{r}) = -\vec{\nabla}\varphi(\vec{r}) + \vec{\nabla} \times \vec{A}(\vec{r}) \,. \tag{4.77}$$

The curl of the vector field $\vec{V}_{\parallel}(\vec{r})$ vanishes as much as the divergence of the vector field $\vec{V}_{\perp}(\vec{r})$. Here, the scalar potential $\varphi(\vec{r})$ is a position-dependent scalar field and the vector potential $\vec{A}(\vec{r})$ is a vector field. In this case,

$$\vec{\nabla} \cdot \vec{V}(\vec{r}) = \vec{\nabla} \cdot \vec{V}_{\parallel}(\vec{r}) = -\vec{\nabla}^2 \varphi(\vec{r}) \tag{4.78a}$$

$$\vec{\nabla} \times \vec{V}(\vec{r}) = \vec{\nabla} \times \vec{V}_{\perp}(\vec{r}) = \vec{\nabla}\left(\vec{\nabla} \cdot \vec{A}(\vec{r})\right) - \vec{\nabla}^2 \vec{A}(\vec{r}) \,. \tag{4.78b}$$

In order to uniquely specify the vector field by a set of differential equations we must give both the curl and divergence of the vector field,

$$\vec{\nabla} \cdot \vec{V}(\vec{r}) = f(\vec{r}) \tag{4.79a}$$

$$\vec{\nabla} \times \vec{V}(\vec{r}) = \vec{j}(\vec{r}) \,, \tag{4.79b}$$

where $f(\vec{r})$ is a scalar field and $\vec{J}(\vec{r})$ is a vector field. In general, any vector field $\vec{V}(\vec{r})$ can be decomposed as

$$\vec{V}(\vec{r}) = \vec{V}_{\parallel}(\vec{r}) + \vec{V}_{\perp}(\vec{r}) \,, \qquad \vec{\nabla} \times \vec{V}_{\parallel}(\vec{r}) = \vec{\nabla} \cdot \vec{V}_{\perp}(\vec{r}) = 0 \,. \tag{4.80}$$

4.2.5 Gauss's Law in Electrodynamics and Faraday's Law

Gauss's law provides the relationship between charged particles and the fields which they generate. This law relates electric fields to electric charge densities, $\rho(\vec{r})$, in the area of electrostatics. We can anticipate here that the same law holds if we assume that the electric field $\vec{E}$ is a function of both position and time,

Gauss's Law: $$\vec{\nabla} \cdot \vec{E}(\vec{r}, t) = \frac{1}{\epsilon_0} \rho(\vec{r}, t) \,, \tag{4.81}$$

which means that Gauss's law holds for electrodynamics as well.

The attentive reader will have noticed that the Eq. (4.68), which states that $\vec{\nabla} \times \vec{E}(\vec{r}) = 0$, is incompatible with the third Maxwell equation (4.1c), which states that

$$\vec{\nabla} \times \vec{E}(\vec{r}, t) = -\frac{\partial}{\partial t} \vec{B}(\vec{r}, t) \,. \tag{4.82}$$

When we state the third Maxwell equation, we assume that the electric field $\vec{E}$ and the magnetic induction $\vec{B}$ are functions of space and time, i.e., $\vec{E} = \vec{E}(\vec{r}, t)$ and $\vec{B} = \vec{B}(\vec{r}, t)$. In Eq. (4.68), however, $\vec{E} = \vec{E}(\vec{r})$ is time-independent. This is the case for electro*statics*, whereas the Maxwell equations deal with electro*dynamics*.

Indeed, it was discovered by Faraday that time-varying magnetic fields would generate an electric field and he developed the relationship, known as Faraday's law. This law is otherwise known as the law of electromagnetic induction.

4.2.6 Magnetostatics and Ampere's Law

Lodestones have been used for millenniums as compass "needles" for navigation. We now understand that the lodestones are magnets. These magnets are aligned by the magnetic field generated by the earth thereby

setting up a north-south reference line. The compass was the principle application of magnetism until the development of electrical batteries which permitted researchers to generate electric currents.

Oersted discovered that magnetic fields were generated by electrical currents. Ampere investigated magnetic forces between charge currents, thereby obtaining a quantitative relationship between charge currents and the magnetic fields they generate. He subsequently proposed a law, Ampere's law, which related magnetic (induction) fields, $\vec{B}\,(\vec{r})$, to electric current densities, $\vec{J}\,(\vec{r})$, in the area of magnetostatics.

Ampere's Law: $$\vec{\nabla} \times \vec{B}\,(\vec{r}) = \mu_0\, \vec{J}\,(\vec{r})\ . \tag{4.83}$$

Here, μ_0 is the magnetic permeability of free space, mesured in henrys per meter. In SI mksA units, J is measured in units of A/m^2.

From Ampere's study of magnetic forces between charge currents it was deduced that the magnetic field exerts a force on moving charged objects. The magnetic force on a charge q, moving with the velocity $\vec{v}$, at a point where the magnetic induction is $\vec{B}$, reads as

$$\vec{F} = q\,\vec{v} \times \vec{B}\,. \tag{4.84}$$

For completeness, we stress that this equation holds in magnetodynamics. In SI mksA units, $\vec{B}$ is measured in Tesla.

4.2.7 Induced Magnetic Fields and the Ampere–Maxwell Law

If taken at face value and generalized to time-dependent magnetic fields and current distributions, Ampere's law becomes inconsistent because it would imply that charge is not conserved. Therefore, the functional form of Ampere's law is in need of an alteration for time-dependent fields. This is demonstrated by the following analysis. It is a mathematical identity that the divergence of the curl of a vector field vanishes,

$$\vec{\nabla} \cdot \left[\vec{\nabla} \times \vec{V}\,(\vec{r})\right] = 0\,, \tag{4.85}$$

where $\vec{V}\,(\vec{r})$ is a vector field. On the one hand, if we apply this identity to Eq. (4.83), we find that ("nothing from nothing means nothing")

$$0 = \vec{\nabla} \cdot \vec{\nabla} \times \vec{B}\,(\vec{r}) = \xi\, 4\pi k_2\, \vec{\nabla} \cdot \vec{J}\,(\vec{r}) = 0\,. \tag{4.86}$$

On the other hand, according to Eq. (4.97), we have that

$$\vec{\nabla} \cdot \vec{J}\,(\vec{r},t) = -\frac{\partial \rho\,(\vec{r},t)}{\partial t}\,. \tag{4.87}$$

These two equations, if they were to hold universally at all times, would imply that the relation

$$\frac{\partial \rho\,(\vec{r},t)}{\partial t} = 0 \tag{4.88}$$

also has to hold, universally. However, this cannot be taken seriously because the term on the right-hand side of Eq. (4.87) is not there by chance. The equation $\vec{\nabla} \cdot \vec{J}\,(\vec{r},t) = -\partial_t \rho\,(\vec{r},t)$ implies that time-varing current densities result in time-varying charge densities. If the local charge density were a constant in time, as implied by Eq. (4.88), then all current configurations in the world would have to be constant in time, which is the case, e.g., for " perfect ring currents". However, in capacitive circuits, when the charge current builds up a charge on the plates of an electrical capacitor, $\rho\,(\vec{r},t)$ manifestly is not a constant on the plates, and

the current furnishing the charge flows from one of the capacitor plates to the other. When the capacitor is fully charged, no more "ring current" flows, and thus $\vec{J} = \vec{J}(\vec{r}, t)$ manifestly is a function of time.

We conclude that Ampere's law therefore cannot hold if we allow charge densities to be time-dependent. Ampere's law correctly describes magnetostatics, i.e., magnetic fields in time-independent current and field configurations. Therefore, we have assumed $\vec{B} = \vec{B}(\vec{r})$ to be a function of $\vec{r}$ in Eq. (4.83). Ampere's law cannot hold if the current configuration is time-dependent, i.e., it cannot correctly describe magnetodynamics, because this would violate charge conservation.

Furthermore, if the current configuration changes over time, then the above consideration suggests to replace the term $\vec{\nabla} \cdot \vec{J}(\vec{r})$ on the right-hand side of (4.86) by the time-dependent expression $\vec{\nabla} \cdot \vec{J}(\vec{r}, t) + \partial_t \rho(\vec{r}, t)$, so that there is no contradiction any more with the conservation of charge. We thus conjecture, according to Maxwell, that

$$\vec{\nabla} \cdot \vec{\nabla} \times \vec{B}\,(\vec{r}, t) = \mu_0 \left[\vec{\nabla} \cdot \vec{J}\,(\vec{r}, t) + \frac{\partial \rho\,(\vec{r}, t)}{\partial t} \right] = 0\,. \tag{4.89}$$

Because Gauss's law given in Eq. (4.81) provides a relationship between charge densities and electric fields, we can replace

$$\rho\,(\vec{r}, t) \to \epsilon_0 \vec{\nabla} \cdot \vec{E}\,(\vec{r}, t) \tag{4.90}$$

on the right-hand side of Eq. (4.86). Then, Eq. (4.86) becomes

$$\begin{aligned} \vec{\nabla} \cdot \left[\vec{\nabla} \times \vec{B}\,(\vec{r}, t) \right] &= \mu_0 \left[\vec{\nabla} \cdot \vec{J}\,(\vec{r}, t) + \epsilon_0 \frac{\partial}{\partial t} \vec{\nabla} \cdot \vec{E}\,(\vec{r}, t) \right] \\ &= \vec{\nabla} \cdot \left[\mu_0\, \vec{J}\,(\vec{r}, t) + \frac{1}{c^2} \frac{\partial}{\partial t} \vec{E}\,(\vec{r}, t) \right] . \end{aligned} \tag{4.91}$$

This guarantees that $\vec{\nabla} \cdot \vec{\nabla} \times \vec{B}\,(\vec{r}) = 0$ and leads to the

Ampere-Maxwell Law: $$\vec{\nabla} \times \vec{B}\,(\vec{r}, t) = \mu_0\, \vec{J}\,(\vec{r}, t) + \frac{1}{c^2} \frac{\partial}{\partial t} \vec{E}\,(\vec{r}, t)\,. \tag{4.92}$$

4.2.8 Absence of Magnetic Monopoles

It is often stated that "magnetic monopoles have never been found" and that this fact is quite fundamental to electromagnetic theory. In the following, we show how to cast this statement into mathematical form. We first remember that Gauss's law Eq. (4.81) and Faraday's law (4.82) determine both the divergence as well as the curl of the electric field,

Electrodynamics for E-Field (SI): $$\vec{\nabla} \cdot \vec{E}(\vec{r}, t) = \frac{1}{\epsilon_0} \rho(\vec{r}, t)\,, \qquad \vec{\nabla} \times \vec{E}(\vec{r}, t) = -\frac{\partial}{\partial t} \vec{B}(\vec{r}, t)\,, \tag{4.93}$$

Electrostatics for E-Field (SI): $$\vec{\nabla} \cdot \vec{E}(\vec{r}) = \frac{1}{\epsilon_0} \rho(\vec{r})\,, \qquad \vec{\nabla} \times \vec{E}(\vec{r}) = 0\,, \tag{4.94}$$

and are thus sufficient to provide a unique boundary value problem for the electric field $E\,(\vec{r}, t)$. When boundary conditions are supplied, then the above equations, given $\rho(\vec{r}, t)$ and $\vec{B}(\vec{r}, t)$, determine $\vec{E}(\vec{r}, t)$ uniquely. By contrast, even when boundary conditions are supplied, the Ampere-Maxwell law by itself does not provide a unique boundary value problem for the magnetic field, because it only determines the curl of the magnetic field.

Thus, Gauss's law, Eq. (4.81), and Faraday's law, Eq. (4.82), uniquely determine the electric field (once boundary conditions are supplied). However, the Ampere-Maxwell law given in (4.92) only gives the curl of

the magnetic field. The same applies for Ampere's law given in Eq. (4.83). It follows that for a given value of the magnetic field on the boundary of some region we can generate many solutions to Eq. (4.92) just by adding a vector $\vec{\nabla}\varphi(\vec{r})$ to $\vec{B}(\vec{r})$ provided that $\vec{\nabla}\varphi(\vec{r})$ vanishes on the boundary. Note that this added vector will not change Eq. (4.83) since $\vec{\nabla}\times\vec{\nabla}\varphi(\vec{r})=\vec{0}$. The additional condition is obtained by requiring that $\vec{\nabla}\cdot\vec{B}(\vec{r})=f(\vec{r})$. In that case, the divergence of the magnetic field, which is equal to $f(\vec{r})$, should be related to the magnetic charge density. Although the search for a magnetic charge continues to this day, none has ever been found. Until magnetic charges have been shown to exist, we assume, as did Maxwell, that

Absence of Magnetic Monopoles: $$\vec{\nabla}\cdot\vec{B}(\vec{r},t)=0 \tag{4.95}$$

in both magnetostatics as well as magnetodynamics.

4.3 Maxwell Equations and Electromagnetic Unit Systems

4.3.1 Summary of Lorentz Force and Maxwell Equations

The four equations (4.81), (4.82), (4.92), and (4.95) were developed and investigated by Ampere, Maxwell, and others in the late 19th century. In modern times, they are known as the Maxwell equations. These equations, together with the force equations, Eq. (4.35) and (4.84), form the basis of classical electrodynamics. Note that the Maxwell equations only determine the time-development of the fields, but they make no statement about the way in which the fields interact with test charges. It is definitely necessary to also specify a force law, and it cannot be derived from the Maxwell equations. Thus, the equations Eq. (4.35) and (4.84), have to be added to form the equation known as the Lorentz force law

Lorentz Force Law: $$\vec{F}=q\left[\vec{E}+k_3\vec{v}\times\vec{B}\right]. \tag{4.96}$$

Furthermore, one of the fundamental conservation laws, namely the conservation of electric charge, also does not follow from the Maxwell equations. This is stated in the relationship between electric charge densities, $\rho(\vec{r})$, and electric current densities, $\vec{J}(\vec{r})$,

Charge Conservation Law: $$\vec{\nabla}\cdot\vec{J}(\vec{r},t)+\frac{\partial\rho(\vec{r},t)}{\partial t}=0. \tag{4.97}$$

4.3.2 Basic Physical Quantities

In the SI system, the Ampere is the unit of current. It measures the time derivative of the charge, $\mathrm{d}q/\mathrm{d}t$, measured in coulombs per second. The vacuum permittivity is

$$\epsilon_0=\frac{10^7}{4\pi c^2}\frac{\mathrm{Am}}{\mathrm{Vs}}=8.854\,187\cdot10^{-12}\,\frac{\mathrm{A\,s}}{\mathrm{V\,m}}=8.854\,187\cdot10^{-12}\,\frac{\mathrm{F}}{\mathrm{m}}. \tag{4.98}$$

The vacuum permeability is

$$\mu_0=4\pi\cdot10^{-7}\,\frac{\mathrm{V\,s}}{\mathrm{A\,m}}=1.256\,637\cdot10^{-6}\,\frac{\mathrm{H}}{\mathrm{m}}. \tag{4.99}$$

Note that the Henry, denoted H, is the SI mksA unit of magnetic inductance. When multiplied by a unit current density of $1\,\mathrm{A\,m^{-2}}$, it gives a magnetic induction field strength of $1\,\mathrm{T}$. An important quantity also is

$$\sqrt{\frac{\mu_0}{\epsilon_0}}=376.730\,313\,\Omega. \tag{4.100}$$

The quantum unit of action is

$$\hbar = 1.0546 \cdot 10^{-34}\,\mathrm{J\,s} = 6.582 \cdot 10^{-16}\,\mathrm{eV\,s}\,. \tag{4.101}$$

The elementary charge is

$$e = 1.602 \cdot 10^{-19}\,\mathrm{C} = 4.803 \cdot 10^{-10}\,\mathrm{statC}\,. \tag{4.102}$$

The fine-structure constant is

$$\alpha = \frac{e^2}{4\pi\epsilon_0\,\hbar\,c} = 137.036^{-1}\,. \tag{4.103}$$

and thus dimensionless. In natural units, the relation becomes particularly simple and instructive, $e^2 = 4\pi\alpha$. The Bohr radius is

$$r_\mathrm{H} = \frac{\hbar}{\alpha\,m_e\,c} = 0.529177\,\mathrm{\AA} = 0.529177 \cdot 10^{-10}\mathrm{m}\,, \tag{4.104}$$

where m_e is the electron mass. In SI mksA units, the ionization energy of atomic hydrogen is

$$\frac{e^2}{4\pi\epsilon_0(2r_\mathrm{H})} = \tfrac{1}{2}\,\alpha^2\,m_e\,c^2 = 13.605\,\mathrm{eV}\,. \tag{4.105}$$

This is the electrostatic potential energy for two elementary charges at a distance equal to two Bohr radii. In Gaussian units, the expression for the ionization energy of atomic hydrogen is a little simpler and reads $e^2/(2r_H)$.

4.4 Electrostatic Energy Density and Self–Energy

4.4.1 Electrostatic Energy Density

Theoretically, we now know how to solve Poisson's equation for the electrostatic potential under arbitrary boundary conditions, for any geometry, and we therefore also know how to calculate the electric field under these circumstances, which is really all we need to know from a physics point of view in order to solve problems in electrostatics. On the other hand, we also know that in order to build up electric (and magnetic) fields, we need to separate positive and negative charges from each other, which requires work. Conversely, a field configuration has the ability to perform work on a test object. How can we formalise these obvious physical facts? The answer to that question will keep us busy for some time now.

Let us define the magnetic field $\vec{H}(\vec{r},t)$, as opposed to the magnetic induction field $\vec{B}(\vec{r},t)$, by the simple relation

$$\vec{H}\,(\vec{r},t) = \frac{1}{\mu_0}\vec{B}(\vec{r},t)\,, \tag{4.106}$$

and the dielectric displacement $\vec{D}(\vec{r},t)$ by the formula

$$\vec{D}(\vec{r},t) = \epsilon_0\,\vec{E}(\vec{r},t)\,. \tag{4.107}$$

Actually, the magnetic field and the dielectric displacement have an additional interpretation if one considers the response of a medium to incoming electromagnetic radiation. However, we will not dwell on this aspect here. Simply, the definition of $\vec{H}$ and $\vec{D}$ simplifies a few derivations below.

Starting with the Maxwell equations, we can first of all obtain the relationship

$$\begin{aligned}\vec{\nabla}\cdot\left[\vec{E}\left(\vec{r},t\right)\times\vec{H}\left(\vec{r},t\right)\right] &= -\vec{E}\left(\vec{r},t\right)\cdot\left[\vec{\nabla}\times\vec{H}\left(\vec{r},t\right)\right]+\vec{H}\left(\vec{r},t\right)\cdot\vec{\nabla}\times\left[\vec{E}\left(\vec{r},t\right)\right]\\ &= -\vec{E}\left(\vec{r},t\right)\cdot\left[\vec{J}\left(\vec{r},t\right)+\frac{\partial}{\partial t}\vec{D}\left(\vec{r},t\right)\right]+\left[\vec{H}\left(\vec{r},t\right)\cdot\left(-\frac{\partial}{\partial t}\vec{B}\left(\vec{r},t\right)\right)\right]\\ &= -\vec{E}\left(\vec{r},t\right)\cdot\vec{J}\left(\vec{r},t\right)-\vec{E}\left(\vec{r},t\right)\cdot\frac{\partial}{\partial t}\vec{D}\left(\vec{r},t\right)-\vec{H}\left(\vec{r},t\right)\cdot\frac{\partial}{\partial t}\vec{B}\left(\vec{r},t\right)\\ &= -\vec{E}\left(\vec{r},t\right)\cdot\vec{J}\left(\vec{r},t\right)-\frac{1}{2}\frac{\partial}{\partial t}\left[\vec{E}\left(\vec{r},t\right)\cdot\vec{D}\left(\vec{r},t\right)+\vec{H}\left(\vec{r},t\right)\cdot\vec{B}\left(\vec{r},t\right)\right]. \end{aligned} \tag{4.108}$$

Without interpretation, this equation is just a meaningless mathematical equality, which reads

$$\vec{\nabla}\cdot\left[\vec{E}\left(\vec{r},t\right)\times\vec{H}\left(\vec{r},t\right)\right]+\vec{E}\left(\vec{r},t\right)\cdot\vec{J}\left(\vec{r},t\right)=-\frac{\partial}{\partial t}\left[\frac{1}{2}\left(\vec{E}\left(\vec{r},t\right)\cdot\vec{D}\left(\vec{r},t\right)+\vec{H}\left(\vec{r},t\right)\cdot\vec{B}\left(\vec{r},t\right)\right)\right]. \tag{4.109}$$

If $\vec{J}(\vec{r},t)$ is to be nonvanishing, then (free) charges have to move. Then, let us assume that $\vec{J}(\vec{r},t)=\Delta q\,\widehat{v}/(\Delta t\,\Delta A)$, where Δq is the charge moving in the time interval Δt through cross-sectional area ΔA, in a direction given by the unit velocity vector $\widehat{v}$. In that case,

$$\vec{E}\left(\vec{r},t\right)\cdot\vec{J}\left(\vec{r},t\right)\approx\frac{\Delta q\,\vec{E}\left(\vec{r},t\right)\cdot\widehat{v}}{\Delta t\,\Delta A}=\frac{\Delta q\,|\vec{E}_{\parallel}|\,\Delta x}{\Delta t\,\Delta V}=\frac{\Delta W}{\Delta t\,\Delta V} \tag{4.110}$$

is the work done on the moving charges per unit time and unit volume. Note that this is the work done by the electric field on the charges, i.e., the work done to accelerate the charges, not the work necessary to move the charges against the electric field. The quantity $\vec{E}\left(\vec{r},t\right)\cdot\vec{J}\left(\vec{r},t\right)$ has the same physical dimension as the time derivative of an energy density. Let us therefore identify

$$\vec{E}\left(\vec{r},t\right)\cdot\vec{J}\left(\vec{r},t\right)=\frac{\partial P\left(\vec{r},t\right)}{\partial V} \tag{4.111}$$

with the local power density corresponding to the work done on the moving charges by the field. Then, we can naturally identify

$$\frac{\partial}{\partial t}u\left(\vec{r},t\right)=\frac{\partial}{\partial t}\frac{1}{2}\left[\vec{E}(\vec{r},t)\cdot\vec{D}(\vec{r},t)+\vec{H}\left(\vec{r},t\right)\cdot\vec{B}\left(\vec{r},t\right)\right], \tag{4.112}$$

$$u\left(\vec{r},t\right)=\frac{1}{2}\left[\vec{E}(\vec{r},t)\cdot\vec{D}(\vec{r},t)+\vec{H}\left(\vec{r},t\right)\cdot\vec{B}\left(\vec{r},t\right)\right], \tag{4.113}$$

where the latter form holds if $\vec{E}$ and $\vec{D}$, and $\vec{H}$ and $\vec{B}$, are strictly proportional to each other. Otherwise, one obtains $u\left(\vec{r},t\right)$ by integrating the defining equation for $\partial_t u\left(\vec{r},t\right)$ with respect to time. Furthermore, $u\left(\vec{r},t\right)$ is the energy density of the electromagnetic field. The time derivative $\partial/\partial t$ then furnishes the right dimension when compared to the other terms in Eq. (4.110). With these identifications, Eq. (4.110) takes (almost) the form of a continuity equation,

$$\vec{\nabla}\cdot\left[\vec{E}\left(\vec{r},t\right)\times\vec{H}\left(\vec{r},t\right)\right]+\frac{\partial u\left(\vec{r},t\right)}{\partial t}+\frac{\partial P\left(\vec{r},t\right)}{\partial V}=0. \tag{4.114}$$

If we now identify the

Poynting vector: $$\vec{S}\left(\vec{r},t\right)=\vec{E}\left(\vec{r},t\right)\times\vec{H}\left(\vec{r},t\right) \tag{4.115}$$

as the energy current density leaving a small test volume, where $\vec{S}$ has the physical dimension of energy per time per area, then we can write

$$\vec{\nabla}\cdot\vec{S}(\vec{r},t)+\frac{\partial u\left(\vec{r},t\right)}{\partial t}+\frac{\partial P\left(\vec{r},t\right)}{\partial V}=0, \tag{4.116}$$

and in view of the divergence theorem,

$$\int_{\partial V} \vec{S}(\vec{r},t)\cdot \mathrm{d}\vec{A} + \int_V \vec{E}(\vec{r},t)\cdot\vec{J}(\vec{r},t)\,\mathrm{d}^3r = -\int_V \frac{\partial u\,(\vec{r},t)}{\partial t}\mathrm{d}^3r\,. \tag{4.117}$$

The interpretation is clear: The rate at which energy leaves a region plus the rate at which field energy is converted to mechanical energy is compensated by a commensurate loss in field energy, i.e., equal to minus the rate at which the field energy changes. $\partial P/\partial V$ is positive when work is done on the charges by the field, i.e., when the work is done "in the direction" of the electromagnetic fields. This work leads to a loss in the energy density. Work done on the charges against the direction of the electromagnetic fields ("actual work") leads to a negative value for $\partial P/\partial V$; and to a positive value for the radiated energy $\int_{\partial V}\vec{S}(\vec{r},t)\cdot\mathrm{d}\vec{A}$ per time.

Let us write the energy dissipation equation (4.116) in a slightly different way,

$$\vec{\nabla}\cdot\vec{S}(\vec{r},t) + \frac{\partial P\,(\vec{r},t)}{\partial V} = -\frac{\partial u\,(\vec{r},t)}{\partial t}\,, \tag{4.118}$$

and compare it to the continuity equation (for the total current)

$$\vec{\nabla}\cdot\vec{J}(\vec{r},t) = -\frac{\partial \rho\,(\vec{r},t)}{\partial t}\,. \tag{4.119}$$

Here, $\vec{J}$ is the current distribution, and ρ is the volume charge density. We can observe the analogy $\vec{S}\leftrightarrow\vec{J}$ and $u\leftrightarrow\rho$. The continuity equation states that a loss in the local charge distribution can only occur if charge leaves the area. The energy dissipation equation states that a loss in the local field energy distribution is compensated when field energy leaves the area (Poynting vector), but the possibility of performing work on the local charges must also be taken into account.

If the field $\vec{E}$ and $\vec{D}$ are always proportional to each other, i.e. they are varied "adiabatically," then we have a unique value for the energy stored by the electromagnetic fields. We will therefore ignore for the present some subtle or not so subtle problems which arise due to frequency dependent relationships between $\vec{E}$ and $\vec{D}$. Before, we have already seen that for time-dependent (notably, rapidly varying) fields, there are convolutions to consider for the relationship of $\vec{E}$ and $\vec{D}$. Note also that a generalization of the concepts presented here to the "mechanical" properties of the electromagnetic field leads to the so-called Maxwell stress tensor, which we will also ignore here.

For electrostatics, which is all we have in mind at this stage, the energy density stored in the electrostatic electric field is

Energy Density: $$w\,(\vec{r}) = \frac{\epsilon_0}{2}\left|\vec{\nabla}\Phi\,(\vec{r})\right|^2\,. \tag{4.120}$$

The electromagnetic energy of a system is given by integrating the energy density over the volume of the system

$$W = \frac{\epsilon_0}{2}\int_V \left|\vec{\nabla}\Phi\,(\vec{r})\right|^2\mathrm{d}^3r \geq 0. \tag{4.121}$$

Let $\rho\,(\vec{r})$ denote the charge density for the system. If the charge density is composed of charge densities for fixed elements, charged point particles, charged surfaces, etc., then it is convenient to express the total charge density as a sum of the individual charge densities

$$\rho\,(\vec{r}) = \sum_i \rho_i\,(\vec{r})\,. \tag{4.122}$$

Each charge density will provide a contribution of the form $-\vec{\nabla}\Phi_i\,(\vec{r})$ to the total electric field at each point where $\vec{\nabla}^2\Phi_i\,(\vec{r}) = -\rho_i\,(\vec{r})\,/\epsilon_0$. In this case,

$$\vec{E}(\vec{r}) = -\vec{\nabla}\Phi\,(\vec{r}) = -\sum_i \vec{\nabla}\Phi_i\,(\vec{r})\,. \tag{4.123}$$

In terms of the fields of the individual charge elements, the electromagnetic energy of the system is

$$\begin{aligned} W &= \frac{\epsilon_0}{2}\int_V \sum_i \vec{\nabla}\Phi_i(\vec{r})\cdot\sum_j \vec{\nabla}\Phi_j(\vec{r})\,\mathrm{d}^3r \\ &= \frac{\epsilon_0}{2}\sum_i\int_V \left|\vec{\nabla}\Phi_i(\vec{r})\right|^2\mathrm{d}^3r + \frac{\epsilon_0}{2}\,2\sum_{i<j}\int_V \vec{\nabla}\Phi_i(\vec{r})\cdot\vec{\nabla}\Phi_j(\vec{r})\,\mathrm{d}^3r\,. \end{aligned} \tag{4.124}$$

The term

$$W_i = \frac{\epsilon_0}{2}\int_V \left|\vec{\nabla}\Phi_i(\vec{r})\right|^2\mathrm{d}^3r \tag{4.125}$$

is the electromagnetic "self energy" of the ith charge element. We can reformulate as follows, provided surface terms vanish (partial integration),

$$\begin{aligned} W_i &= \frac{\epsilon_0}{2}\int_V \left(\vec{\nabla}\Phi_i(\vec{r})\right)^2\mathrm{d}^3r = -\frac{\epsilon_0}{2}\int_V \Phi_i(\vec{r})\;\vec{\nabla}^2\Phi_i(\vec{r})\mathrm{d}^3r \\ &= -\frac{\epsilon_0}{2}\int_V \mathrm{d}^3r\left(\frac{1}{4\pi\epsilon_0}\int_V \mathrm{d}^3r'\frac{1}{|\vec{r}-\vec{r}'|}\,\rho_i(\vec{r}')\right)\left(-\frac{1}{\epsilon_0}\rho_i(\vec{r})\right) \\ &= \frac{1}{8\pi\epsilon_0}\int_V \mathrm{d}^3r\int_V \mathrm{d}^3r'\rho_i(\vec{r})\frac{1}{|\vec{r}-\vec{r}'|}\,\rho_i(\vec{r}')\;, \end{aligned} \tag{4.126}$$

which is some sort of generalization of Coulomb's law. As long as the charge density of the element does not change this "self energy" will be fixed. The second term,

$$W_{ij} = \epsilon_0\int_V \vec{\nabla}\Phi_i(\vec{r})\cdot\vec{\nabla}\Phi_j(\vec{r})\,\mathrm{d}^3r, \tag{4.127}$$

with $i \neq j$, provides the interaction energy between the charged elements. Again, provided surface terms vanish, we can write

$$W_{ij} = \frac{1}{4\pi\epsilon_0}\int_V \mathrm{d}^3r\int_V \mathrm{d}^3r'\rho_i(\vec{r})\frac{1}{|\vec{r}-\vec{r}'|}\,\rho_j(\vec{r}')\;. \tag{4.128}$$

The significance of the self energy and interaction energy is illustrated by the following example.

4.4.2 Example of Self Energy and Interaction Energy

Consider two identical non-conducting spherical shells (which ensures that we do not need to consider a rearrangement of charge on the shells as they approach each other). Let each have a radius a and let their centers be separated by a distance $R \geq 2a$. The surface charge density of one shell is σ_0, and the surface charge of the other is -σ_0. We investigate the self energy of each spherical shell and the interaction energy of the spherical shells.

The magnitude of the charge on each shell is $q = 4\pi a^2\sigma_0$. The electric field of the spherical shell vanishes inside the shell while outside the shell the electric field is

$$\vec{E}(\vec{r}-\vec{r}_\pm) = \frac{\pm q\;(\vec{r}-\vec{r}_\pm)}{4\pi\epsilon_0\,|\vec{r}-\vec{r}_\pm|^3} = -\vec{\nabla}\Phi_\pm(\vec{r})\,. \tag{4.129}$$

To calculate the self energy of each shell, we evaluate

$$W_0 = \frac{\epsilon_0}{2}\int_{\mathbb{R}^3}\left|\vec{E}(\vec{r})\right|^2\mathrm{d}^3r = \frac{\epsilon_0\,q^2}{2(4\pi\epsilon_0)^2}\int_{|\vec{r}-\vec{r}_\pm|>a}\frac{\mathrm{d}^3r}{|\vec{r}-\vec{r}_\pm|^4}. \tag{4.130}$$

For each shell we can let $\vec{r}' = \vec{r} - \vec{r}_\pm$ (or alternatively center the spheres at the origin because the self energy is translation invariant). Then, the self energy of each spherical shell is found to be

$$\begin{aligned} W_0 &= \frac{\epsilon_0 q^2}{2(4\pi\epsilon_0)^2} \int_{|\vec{r}'|>a} \frac{\mathrm{d}^3 r'}{|\vec{r}'|^4} = \frac{4\pi\,\epsilon_0 q^2}{2(4\pi\epsilon_0)^2} \int_a^\infty \frac{1}{r'^2}\mathrm{d}r' \\ &= \frac{q^2}{2\cdot 4\pi\epsilon_0}\left[-\frac{1}{r'}\right]_a^\infty = \frac{q^2}{8\pi\epsilon_0\, a}\,. \end{aligned} \tag{4.131}$$

Detour: Start. We can use this result in order to estimate the charge radius of the electron. Suppose we consider the electron to be a spherical charged shell. In this case the electromagnetic energy stored in the electric field of the electron would be

$$W_e = \frac{e^2}{8\pi\epsilon_0\, a}\,. \tag{4.132}$$

The total energy of an electron at rest is $m_e c^2$. The question now is what would be the radius of the electron if all its energy was equal to the energy stored by the electric field?

The classical electron radius obtained when equating the observed mass/energy of the electron with the electrostatic self energy of a spherical shell, is obtained as

$$a = 1.4\times 10^{-13}\mathrm{cm}\,. \tag{4.133}$$

If this were correct, then the electron radius would be of the same order of magnitude as the observed proton radius. If the electron were an even smaller spherical shell, then its electrostatic self energy would be even larger. However, the upper limit on the radius of the electron is several orders of magnitude below the radius of the proton. In fact the results of all experiments at this time are consistent with the electron being a point particle! What happened to its electromagnetic energy?

Well, from a quantum point of view, the electron never knows where it actually is. Heisenberg's uncertainty principle states that once we know the position of the electron precisely, then we do not know its momentum at all, and it could be moving at maximum speed "with respect to itself," questioning the concept of the electrostatic self energy. We cannot define the location of an electron precisely, but from the point of view of quantum mechanics, we can know its probability density $|\psi(\vec{r})|^2$, where $\psi(\vec{r})$ is the complex probability amplitude (not density!) of the electron wave function at point $\vec{r}$. Its charge density then is $\rho(\vec{r}) = e\,|\psi(\vec{r})|^2$, and according to the above arguments, its electrostatic energy might be assumed to be given by the expression

$$W_{\mathrm{guess}} = \frac{1}{8\pi\epsilon_0}\int \mathrm{d}^3 r \int \mathrm{d}^3 r'\,\rho(\vec{r})\frac{1}{|\vec{r}-\vec{r}'|}\,\rho(\vec{r}') = \frac{e^2}{8\pi\epsilon_0}\int \mathrm{d}^3 r \int \mathrm{d}^3 r'\,|\psi(\vec{r})|^2\frac{1}{|\vec{r}-\vec{r}'|}|\psi(\vec{r}')|^2\,. \tag{4.134}$$

Indeed, similar expressions result from the theory of quantum electrodynamics for the self-energy of the electron, but the electrostatic self energy is supplemented there by many more terms, some of which are of dynamic origin. In order to fully understand this problem, one also has to quantize the electromagnetic field into so-called photons. Indeed, when these static and dynamic terms are written down for a pointlike, bound electron, then the self-energy of the bound electron diverges in analogy to the above self-energy integrals which also diverge if one assumes that the electron is a point-like particle. In order to see this, take the limit $a \to 0$ in Eq. (4.132). This is in contrast to the observed rest mass of the electron which is finite and equal to $0.511\,\mathrm{MeV}/c^2$, where $1\,\mathrm{MeV} = 10^6\,\mathrm{eV}$ where $1\,\mathrm{eV} = 1.602\times 10^{-19}\mathrm{J}$. However, the divergence of the bound-electron self energy is only logarithmic in a cutoff parameter (the cutoff parameter is the energy of the exchanged so-called virtual photon that the charge cloud of the electron exchanges with itself). Now, since the divergence is only logarithmic, Hans A. Bethe in 1947 suggested that one might identify a part of that divergent self energy with the mass of the particle and interpret the rest of the energy shift as an explanation of an experiment performed by Willis E. Lamb in the same year. The original idea is similar to

the one which we shall discuss in the following, in order to regularize and renormalize the potential of a long charged long wire. The theory of quantum electrodynamics had stood its first test, and one of the most intriguing concepts of modern physics was born: the renormalization. Today, the renormalization of the bound-electron self energy is carried out routinely by field theorists, and spectral lines in simple atomic systems like hydrogen or helium are being compared to experiment on the level of one part in 10^{14}. *Detour: End.*

The potential due to a uniform spherical shell of charge centered at the origin is

$$\begin{aligned} \Phi_\pm(\vec{r}) &= \frac{\pm q}{4\pi\epsilon_0 r} \qquad \text{for } r > a\,, \\ \Phi_\pm(\vec{r}) &= \frac{\pm q}{4\pi\epsilon_0 a} \qquad \text{for } r \leq a\,, \end{aligned} \tag{4.135}$$

where q is the total charge of the shell and a is the radius of the shell. Let us denote by $\vec{r}_+$ and $\vec{r}_-$ the centers of the two spheres. Then, in terms of this potential, the interaction energy stored by the electric field is

$$W_{\rm int} = \epsilon_0 \int_{\mathbb{R}^3} \vec{\nabla}\Phi_+(\vec{r}-\vec{r}_+)\cdot\vec{\nabla}\Phi_-(\vec{r}-\vec{r}_-)\,{\rm d}^3r\,. \tag{4.136}$$

Using the identity

$$\vec{\nabla}\cdot\Big[\Phi_+(\vec{r}-\vec{r}_+)\,\vec{\nabla}\Phi_-(\vec{r}-\vec{r}_-)\Big] = \vec{\nabla}\Phi_+(\vec{r}-\vec{r}_+)\cdot\vec{\nabla}\Phi_-(\vec{r}-\vec{r}_-) + \Phi_+(\vec{r}-\vec{r}_+)\,\vec{\nabla}^2\Phi_-(\vec{r}-\vec{r}_-)\,, \tag{4.137}$$

or alternatively by an integration by parts, we can write

$$W_{\rm int} = -\epsilon_0 \int_{\mathbb{R}^3} \Phi_+(\vec{r}-\vec{r}_+)\,\vec{\nabla}^2\Phi_-(\vec{r}-\vec{r}_-)\,{\rm d}^3r\,. \tag{4.138}$$

Now, we let $\vec{r}' = \vec{r}-\vec{r}_-$ and write

$$W_{\rm int} = -\epsilon_0 \int_{\mathbb{R}^3} \Phi_+(\vec{r}'-\vec{r}_++\vec{r}_-)\,\vec{\nabla}^2\Phi_-(\vec{r}')\,{\rm d}^3r'\,. \tag{4.139}$$

The surface of $\mathbb{R}^3$ is a large sphere of radius r_s' with $r_s' \to \infty$. Since the product of the field and the potential vanish at infinity as $r_s'^{-3}$ whereas the surface area $\int {\rm d}\vec{S}'$ only increases like $r_s'^2$, the surface integral does not contribute to the interaction energy. To evaluate the spatial integration, we choose a configuration where $\vec{\nabla}^2\Phi(\vec{r}')$ refers to the negative shell. The charge density on the negative shell, therefore, fulfills the equation

$$\vec{\nabla}^2\Phi_-(\vec{r}') = -\frac{1}{\epsilon_0}\,\rho_-(\vec{r}) = -\frac{1}{\epsilon_0}\,(-\sigma_0)\,\delta(r'-a)\,, \tag{4.140}$$

where $\sigma_0 = q/(4\pi a^2)$ is the magnitude of the charge density on the oppositely charged shells (we assume $q>0$). Here, we have used the fact that the charge density of the spherical shell is located on the surface of the spherical shell, and that $|\vec{\nabla}r| = 1$. The equation of the sphere, which is $r' = a$ in spherical coordinates, therefore leads to

$$\rho_+(\vec{r}') = \sigma_0\,\delta(r'-a)\,|\vec{\nabla}'(r'-a)| = \sigma_0\,\delta(r'-a)\,, \tag{4.141}$$

confirming the result given previously. In the example, the distance between the centers of the spheres is greater than the diameter of the spheres. We set

$$\vec{r}_+ - \vec{r}_- = \vec{R} = R\,\hat{\rm e}_z \tag{4.142}$$

and assume that the separation of the spheres is along the z axis. Because the spheres do not overlap, the interaction energy is given by

$$\begin{aligned} W_{\rm int} &= -\epsilon_0 \int_{\mathbb{R}^3} \Phi_+ \left(\vec{r}' - \vec{r}_+ + \vec{r}_-\right) \vec{\nabla}^2 \Phi_- \left(\vec{r}'\right) {\rm d}^3 r' \\ &= -\epsilon_0 \int_{\mathbb{R}^3} \frac{q}{4\pi\epsilon_0 |\vec{r}' - (\vec{r}_+ - \vec{r}_-)|} \left[-\frac{(-\sigma_0)}{\epsilon_0} \delta\left(r' - a\right) \right] {\rm d}^3 r' \\ &= -\frac{q\,\sigma_0}{\epsilon_0} \frac{1}{4\pi} \int_0^\pi \int_0^\infty \int_0^{2\pi} \frac{\delta\left(r' - a\right)}{\left[r'^2 + R^2 - 2r'\,R\,\cos\theta\right]^{1/2}} \, {\rm d}\varphi \, r'^2 {\rm d}r' \, \sin\theta \, {\rm d}\theta \,. \end{aligned} \tag{4.143}$$

The integration over the angle $\int_0^{2\pi} {\rm d}\varphi = 2\pi$ and the radial direction r are readily carried out,

$$W_{\rm int} = -\frac{q\,\sigma_0}{\epsilon_0} \frac{2\pi}{4\pi} \int_0^\pi \frac{a^2}{\left[a^2 + R^2 - 2aR\cos\theta\right]^{1/2}} \, \sin\theta \, {\rm d}\theta \,. \tag{4.144}$$

This leaves the integral over θ. Using $\sigma_0 = q/(4\pi a^2)$ and the substitution $\xi = \cos\theta$, we obtain

$$\begin{aligned} W_{\rm int} &= -\frac{q\left[\frac{q}{4\pi a^2}\right] a^2}{2\epsilon_0} \int_{-1}^{+1} \frac{{\rm d}\xi}{\left[a^2 + R^2 - 2aR\xi\right]^{1/2}} \\ &= -\frac{q^2}{2\cdot 4\pi\epsilon_0} \int_{\xi=-1}^{\xi=+1} \left(-\frac{1}{a\,R} {\rm d}\left[a^2 + R^2 - 2aR\xi\right]^{1/2} \right) \\ &= \frac{q^2}{2\cdot 4\pi\epsilon_0} \frac{[R-a] - [R+a]}{aR} = -\frac{q^2}{4\pi\epsilon_0 R} \,, \end{aligned} \tag{4.145}$$

which is our result for the interaction energy of two shells. The interaction energy is equal to that of two charged point particles, with charges $\pm q$, separated by a distance R. The total energy stored in the electrostatic field is

$$W = 2W_0 + W_{\rm int} = 2 \times \frac{q^2}{8\pi\epsilon_0 a} - \frac{q^2}{4\pi\epsilon_0 R} > 0 = \frac{q^2}{4\pi\epsilon_0} \left(\frac{1}{a} - \frac{1}{R} \right) , \tag{4.146}$$

where we recall the result (4.131). As the separation R increases, the term

$$-\frac{q^2}{4\pi\epsilon_0 R} \tag{4.147}$$

increases, and the stored energy increases. For an infinitesimal change ${\rm d}R$ in the separation, the change in the interaction energy is given by

$${\rm d}W = {\rm d}R \, \frac{\partial}{\partial R} \left[-\frac{q^2}{4\pi\epsilon_0 R} \right] = \frac{q^2}{4\pi\epsilon_0 R^2} \, {\rm d}R = -F_C \, {\rm d}R \,, \tag{4.148}$$

where F_C is the Coulomb attractive force between the spheres which attracts the two oppositely charged spheres toward each other. If we increase the distance infinitesimally by ${\rm d}R$, then work needs to be done against the attractive Coulomb force whose component in the radial direction is F_C, hence the minus sign. According to Eq. (4.148), when the spheres approach each other (${\rm d}R < 0$), the field energy decreases, ${\rm d}W < 0$. However, as the spheres move toward each other, the Coulomb force does mechanical work ${\rm d}W_C$, where

$${\rm d}W_C = -{\rm d}W = F_C \, {\rm d}R = -\frac{q^2}{4\pi\epsilon_0 R^2} \, {\rm d}R > 0 \qquad \text{for } {\rm d}R < 0, \tag{4.149}$$

on the spheres, thus compensating the loss in field energy that occurs when the distance among the spheres decreases. In practice, the spheres would be accelerated toward each other by the attractive Coulomb force at the same time as the field energy descreases.

Chapter 5

Multipole Decompositions

5.1 Highly Nontrivial Charge Distributions in the Far Field

5.1.1 Spherical Coordinates

Let us remember, from PHYSICS 6403 or elsewhere, the expressions for the gradient, Laplacian and curl in spherical coordinates. We have for the gradient,

$$\vec{\nabla}\Phi = \hat{e}_r \, \frac{\partial \Phi}{\partial r} + \hat{e}_\theta \, \frac{1}{r} \frac{\partial \Phi}{\partial \theta} + \hat{e}_\varphi \, \frac{1}{r \, \sin\theta} \frac{\partial \Phi}{\partial \varphi} \, . \tag{5.1}$$

Let us also consider a vector field in spherical coordinates, with unit vectors $\hat{e}_{(r)}$, $\hat{e}_{(\theta)}$, and $\hat{e}_{(\varphi)}$ (compare with the covariant and contravariant basis vectors in PHYSICS 6403), in the radial, polar and azimuthal directions. Here, one has the decomposition

$$\vec{A} = A_{(r)} \, \hat{e}_{(r)} + A_{(\theta)} \, \hat{e}_{(\theta)} + A_{(\varphi)} \, \hat{e}_{(\varphi)} \, . \tag{5.2}$$

The divergence is given as

$$\begin{aligned} \vec{\nabla} \cdot \vec{A} = \; & = \frac{1}{r^2 \, \sin\theta} \frac{\partial}{\partial r} \, \left(r^2 \, \sin\theta \, A_{(r)} \right) + \frac{1}{r^2 \, \sin\theta} \frac{\partial}{\partial \theta} \, \left(r \, \sin\theta \, A_{(\theta)} \right) + \frac{1}{r^2 \, \sin\theta} \frac{\partial}{\partial \varphi} \, \left(r \, A_{(\varphi)} \right) \\ & = \frac{1}{r^2} \frac{\partial}{\partial r} \, \left(r^2 \, A_{(r)} \right) + \frac{1}{r \, \sin\theta} \frac{\partial}{\partial \theta} \, \left(\sin\theta \, A_{(\theta)} \right) + \frac{1}{r \, \sin\theta} \frac{\partial}{\partial \varphi} \, A_{(\varphi)} \, . \end{aligned} \tag{5.3}$$

This form clarifies the form of the divergence for a vector field.

The Laplacian is

$$\begin{aligned} \vec{\nabla}^2 \Phi = & \frac{1}{r^2 \, \sin\theta} \, \partial_r (r^2 \, \sin\theta \, \partial_r \Phi) + \frac{1}{r^2 \, \sin\theta} \, \partial_\theta (\sin\theta \, \partial_\theta \Phi) + \frac{1}{r^2 \, \sin\theta} \, \partial_\varphi \left(\frac{1}{\sin\theta} \partial_\varphi \Phi \right) \\ = & \frac{1}{r^2} \, \partial_r (r^2 \, \partial_r \Phi) + \frac{1}{r^2 \, \sin\theta} \, \partial_\theta (\sin\theta \, \partial_\theta \Phi) + \frac{1}{r^2 \, \sin^2\theta} \, \partial_\varphi^2 \Phi \, . \end{aligned} \tag{5.4}$$

The curl is

$$\begin{aligned}\vec{\nabla}\times\vec{A} = & = \frac{1}{r^2\sin\theta}\left[\partial_\theta\left(r\,\sin\theta\,A_{(\varphi)}\right)-\partial_\varphi\left(rA_{(\theta)}\right)\right]\,\hat{e}_{(r)}\\ & + \frac{1}{r\,\sin\theta}\left[\partial_\varphi\left(A_{(r)}\right)-\partial_r\left(r\,\sin\theta\,A_{(\varphi)}\right)\right]\,\hat{e}_{(\theta)}\\ & + \frac{1}{r}\left[\partial_r\left(rA_{(\theta)}\right)-\partial_\theta A_{(r)}\right]\,\hat{e}_{(\varphi)}\\ & = \frac{1}{r\sin\theta}\left[\partial_\theta\left(\sin\theta\,A_{(\varphi)}\right)-\partial_\varphi A_{(\theta)}\right]\,\hat{e}_{(r)}\\ & + \frac{1}{r\,\sin\theta}\left[\partial_\varphi A_{(r)}-\sin\theta\,\partial_r\left(r\,A_{(\varphi)}\right)\right]\,\hat{e}_{(\theta)}\\ & + \frac{1}{r}\left[\partial_r\left(rA_{(\theta)}\right)-\partial_\theta A_{(r)}\right]\,\hat{e}_{(\varphi)}\,. \end{aligned} \tag{5.5}$$

These formulas are recorded in Eqs. (13.8), (13.29), (13.52), and (13.61) of the scriptum notes in PHYSICS 6403.

5.1.2 Laplace Equation in Spherical Coordinates

General Solution to the Homogeneous Equation. The Poisson equation is the Laplace equation almost everywhere (except at the source). We therefore start with the Laplace equation. We use the Laplace equation in spherical coordinates (r,θ,φ) has the form

$$\begin{aligned}\vec{\nabla}^2\Phi = & \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}\,\Phi\left(r,\theta,\varphi\right)\right]-\frac{1}{r^2}\left\{\vec{L}\cdot\vec{L}\right\}\Phi\left(r,\theta,\varphi\right)\\ & = \frac{1}{r}\frac{\partial^2}{\partial r^2}r\,\Phi\left(r,\theta,\varphi\right)-\frac{1}{r^2}\vec{L}^2\,\Phi\left(r,\theta,\varphi\right)\\ & = \frac{\partial^2}{\partial r^2}\,\Phi\left(r,\theta,\varphi\right)+\frac{2}{r}\,\frac{\partial}{\partial r}\,\Phi\left(r,\theta,\varphi\right)-\frac{1}{r^2}\vec{L}^2\,\Phi\left(r,\theta,\varphi\right)=0\\ & = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\,\Phi\left(r,\theta,\varphi\right)+-\frac{1}{r^2}\vec{L}^2\,\Phi\left(r,\theta,\varphi\right)=0\,, \end{aligned} \tag{5.6}$$

where the square of the angular momentum operator

$$\vec{L} = -\mathrm{i}\vec{r}\times\vec{\nabla} \tag{5.7}$$

is equal to

$$-\vec{L}^2 \equiv \left(\vec{r}\times\frac{\partial}{\partial\vec{r}}\right)^2 = \left(\vec{r}\times\vec{\nabla}\right)^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\,. \tag{5.8}$$

Various forms of the radial part of the Laplacian operator have been used. Remark: In quantum mechanics, the angular momentum operator is defined as

$$\vec{L} = \vec{r}\times\vec{p} = \vec{r}\times\left(-\mathrm{i}\hbar\vec{\nabla}\right)\,, \tag{5.9}$$

and is equal to our $\vec{L}$ provided we set $\hbar=1$, and/or provided we scale the $\vec{L}$ operator by a factor $\hbar^{-1}$. In order to separate angular and radial variables, we multiply Eq. (5.6) by r^2 and use the ansatz

$$\Phi\left(r,\theta,\varphi\right) = R\left(r\right)Y\left(\theta,\varphi\right), \tag{5.10}$$

and obtain

$$\frac{1}{R(r)}\left\{\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}\,R(r)\right]\right\} = \frac{1}{Y(\theta,\varphi)}\vec{L}^2\,Y(\theta,\varphi)\,. \tag{5.11}$$

This equation must be satisfied for all (r,θ,φ). As (r,θ,φ) are independent variables, Eq. (5.11) can only be satisfied if both sides equal a constant which we choose as $\ell(\ell+1)$. Then,

$$\vec{L}^2\,Y(\theta,\varphi) = \ell\,(\ell+1)\,Y(\theta,\varphi)\,, \tag{5.12}$$

and the radial part of the function fulfills

$$\frac{\mathrm{d}}{\mathrm{d}r}\left[r^2\frac{\mathrm{d}}{\mathrm{d}r}R(r)\right] - \ell(\ell+1)R(r) = 0\,. \tag{5.13}$$

Equation (5.12) can be further separated using the separation ansatz $Y(\theta,\varphi) = V(\theta)W(\varphi)$:

$$\frac{1}{V(\theta)}\sin\theta\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}V(\theta)\right] + \frac{1}{V(\theta)}\,\sin^2\theta\,\ell(\ell+1)\,V(\theta) = -\frac{1}{W(\varphi)}\,\frac{\partial^2}{\partial\varphi^2}W(\varphi)\,. \tag{5.14}$$

Again, since θ and φ are independent variables, both sides must equal a constant (the second separation constant) which we take to be $-m^2$ and write

$$\frac{\partial^2}{\partial\varphi^2}\,W(\varphi) = -m^2\,W(\varphi) \qquad \Rightarrow \qquad W_m(\varphi) = A_m\,\mathrm{e}^{\mathrm{i}m\varphi} + B_m\,\mathrm{e}^{-\mathrm{i}m\varphi} \tag{5.15}$$

and so

$$\sin\theta\frac{\partial}{\partial\theta}\,\left[\sin\theta\frac{\partial}{\partial\theta}\,V(\theta)\right] + \left\{\sin^2\theta\,\ell(\ell+1) - m^2\right\}\,V(\theta) = 0\,. \tag{5.16}$$

Substituting $u = \cos\theta$, Eq. (5.16) becomes the associated Legendre equation:

$$\frac{\mathrm{d}}{\mathrm{d}u}\left[(1-u^2)\,\frac{\mathrm{d}}{\mathrm{d}u}F(u)\right] + \left\{\ell\,(\ell+1) - \frac{m^2}{1-u^2}\right\}\,F(u) = 0\,, \qquad u = \cos\theta\,, \tag{5.17}$$

with two linearly independent solutions called the associated Legendre functions of the first, $P_\ell^{|m|}(u)$, and second kind, $Q_\ell^{|m|}(u)$. The general solution to the polar equation reads as

$$F_{\ell,m}(u) = A_{\ell,m}\,P_\ell^m(u) + B_{\ell,m}\,Q_\ell^m(u)\,. \tag{5.18}$$

For $-\ell < m \le \ell$, with $\ell = 0,1,2,\ldots$, the $P_\ell^m(\cos\theta)$ are finite in the interval $0 \le \theta \le \pi$. By contrast, the $Q_\ell^m(\cos\theta)$ diverge at $u = \cos\theta = \pm 1$ or $\theta = 0,\pi$ (i.e., on the "pole caps" of the unit sphere). While the $Q_\ell^m(\cos\theta)$ are possible solutions when we can manifestly restrict the range of allowed polar angles to $|\cos\theta| < 1$, we must exclude these solutions if we seek functions that converge to finite values on the entire unit sphere. The functions $P_\ell^m(u)$ and $P_\ell^{-m}(u)$ are not linearly independent, but rather, directly proportional to each other,

$$P_\ell^{-|m|}(u) = (-1)^{|m|}\,\frac{(\ell-|m|)!}{(\ell+|m|)!}\,P_\ell^{|m|}(u)\,. \tag{5.19}$$

Given a solution $F_{\ell,m}(u)$, the integration constants $A_{\ell,m}$ and $B_{\ell,m}$ are thus not uniquely determined, but the form of the solution given in Eq. (5.18) is still general.

We shall assume that the solution $\Phi = \Phi(r,\theta,\varphi)$ of the Laplace equation is well defined on the entire unit sphere and write the general solution to the homogeneous equation as

$$\Phi(r,\theta,\varphi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\left(a_{\ell,m}\,r^\ell + b_{\ell,m}\,r^{-\ell-1}\right)\,P_\ell^m(\cos\theta)\,e^{\mathrm{i}m\varphi}\,, \tag{5.20}$$

with arbitrary constants $a_{\ell,m}$ and $b_{\ell,m}$. We have absorbed the integration constants $A_{\ell,m}$ and $B_{\ell,m}$ into the coefficients $a_{\ell,m}$ and $b_{\ell,m}$ which multiply the radial factors. From Eq. (5.15), we might otherwise assume that the allowed range for m contains the entire set of the positive and negative integers, and zero. However, the m in Eq. (5.15) has to be the same as the one in Eq. (5.18), and the associated Legendre polynomials $P_\ell^m(\cos\theta)$ are well-defined only for $-\ell < m \leq \ell$. Furthermore, the $P_\ell^m(u)$ and $P_\ell^{-m}(u)$ are not linearly independent, and it turns out that we can formulate the general form of the homogeneous solution using factors $e^{\mathrm{i}m\varphi}$, with $-\ell < m < \ell$.

Based on Eq. (5.20), we may proceed to solve the inhomogeneous equation defining the Green function by matching the solution regular at the origin (r^ℓ) with the solution regular at infinity ($r^{-\ell-1}$) near the turning point, where the Dirac δ function is nonvanishing. However, before we proceed to this endeavour, we first dwell a little on the Legendre functions, and spherical harmonics, which constitute examples of "special functions" which are so important in mathematical physics.

Legendre Functions of the First Kind. In our problem, we expect the functions to be well behaved for all $|u| = |\cos\theta| \leq 1$. A special case is found when $|m| = 0$. These solutions,

$$P_\ell^0(u) = P_\ell(u)\,, \tag{5.21}$$

are called Legendre functions or Legendre polynomials. The first few $P_\ell\,(u) = P_\ell^0(u)$ read

$$P_0\,(u) = 1\,, \qquad P_1\,(u) = u\,, \tag{5.22a}$$

$$P_2\,(u) = \frac{1}{2}\left(3u^2 - 1\right)\,, \tag{5.22b}$$

$$P_3\,(u) = \frac{u}{2}\left(5u^2 - 3\right)\,, \tag{5.22c}$$

$$P_4\,(u) = \frac{1}{8}\left(35u^4 - 30u^2 + 3\right)\,. \tag{5.22d}$$

The associated Legendre polynomials $P_\ell^{|m|}(u) \equiv P_\ell^m(u)$ of degree ℓ and order m are related to the Legendre polynomials by

$$P_\ell^m\,(u) = (-1)^m\,\left(1-u^2\right)^{m\,/\,2}\,\frac{\mathrm{d}^m P_\ell\,(u)}{\mathrm{d}u^m}\,, \qquad m \geq 0\,; \tag{5.23a}$$

$$P_\ell^{-m}\,(u) = (-1)^m\,\frac{(\ell-m)!}{(\ell+m)!}\,P_\ell^m\,(u)\,. \qquad \text{transformation } m>0 \text{ to } m<0\,. \tag{5.23b}$$

This particular sign convention is just one possibility. Because $P_\ell\,(u)$ is a polynomial of order ℓ, these are only non-zero when $\ell \geq |m|$. There are orthogonality relations,

$$\int_{-1}^{1} \mathrm{d}u\, P_{\ell'}^m(u)\, P_\ell^m(u) = \frac{2}{2\ell+1}\,\frac{(\ell+m)!}{(\ell-m)!}\,\delta_{\ell\,\ell'}\,. \tag{5.24}$$

Finally, we note that at $P_\ell^0\,(1) = 1$ (by definition), $P_\ell^0\,(-1) = (-1)^\ell$, and if $m \neq 0$, $P_\ell^m\,(\pm 1) = 0$. The general symmetry relation of these functions for $u \to -u$ is

$$P_\ell^m\,(-u) = (-1)^{\ell+m}\;P_\ell^m\,(u)\,. \tag{5.25}$$

Legendre Functions of the Second Kind. The irregular solutions are the Legendre functions of the second kind, which are the functions $Q_\ell\,(u)$ that have singularities at $u = \pm 1$. The Legendre functions of

the second kind can be expressed as follows ($|u| \leq 1$),

$$Q_n\,(u) = \frac{P_n(u)}{2} \ln\left(\frac{1+u}{1-u}\right) + \mathcal{Q}_n(u) = P_n(u)\,\mathrm{arctanh}\,(u) + \mathcal{Q}_n(u)\,, \tag{5.26a}$$

$$\mathcal{Q}_0\,(u) = 0\,, \qquad \mathcal{Q}_1\,(u) = -1\,, \qquad \mathcal{Q}_2\,(u) = -\frac{3}{2}\,u\,, \qquad \mathcal{Q}_3\,(u) = -\frac{5}{2}\,u^2 + \frac{2}{3}\,. \tag{5.26b}$$

We note the logarithmic divergences for $Q_n\,(u)$ at $u \to \pm 1$.

In order to find a generalizated expression for the associated Legendre functions, we have to dwell a little into the definition of an ominous function of mathematical physics, so called complete (Gaussian) hypergeometric function. Who's afraid of the hypergeometric function? In order to understand this function, we remember that a so called geometric series is a series of terms

$$\sum_{n=0}^{\infty} z^n = \frac{1}{1-z}\,. \tag{5.27}$$

When we decorate all the terms in that series by appropriate prefactors, we get

$${}_2F_1(a,b,c;z) = \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(a)}\,\frac{\Gamma(b+n)}{\Gamma(b)}\,\frac{\Gamma(c)}{\Gamma(c+n)}\,\frac{z^n}{n!}\,, \tag{5.28}$$

where

$$\Gamma(z) = \int_0^{\infty} t^{z-1}\,\exp(-t)\,\mathrm{d}t\,, \qquad\qquad \Gamma(n) = (n-1)!\,. \tag{5.29}$$

In particular, we have as a special case of the (hyper-)geometric function,

$${}_2F_1(1,1,1;z) = \sum_{n=0}^{\infty} \frac{\Gamma(1+n)}{\Gamma(1)}\,\frac{\Gamma(1+n)}{\Gamma(1)}\,\frac{\Gamma(1)}{\Gamma(1+n)}\,\frac{z^n}{n!} = \sum_{n=0}^{\infty} z^n = \frac{1}{1-z}\,. \tag{5.30}$$

For zero or negative integer first argument $a = -m$ of the hypergeometric function ${}_2F_1(a,b,c;z)$, we have the following situation. When the index $n \leq m$, we have two Γ functions of negative argument in the expression $\Gamma(a+n)/\Gamma(a) = \Gamma(-m+n)/\Gamma(-m)$. On the other hand, when $n > m$, then the expression $\Gamma(a+n)/\Gamma(a) = \Gamma(-m+n)/\Gamma(-m) = 0$, because the denominator is infinite, whereas the numerator is finite. The series thus terminates at summation index $n = m$. In general, the associated Legendre functions can be written in terms of the hypergeometric function ${}_2F_1(a,b,c;z)$, which is an infinite series that terminates for a (or b) equal to a negative integer. The termination of the series for $a = m - \ell$ produces the convergence of the $P_\ell^m\,(u)$:

$$Q_\ell^m\,(u) = \text{constant} \;\times\; \left(\frac{u+1}{u-1}\right)^{m/2} {}_2F_1\left(-\ell, \ell+1, 1-m; \frac{1-u}{2}\right)\,, \tag{5.31a}$$

$$P_\ell^m\,(u) = \text{constant} \;\times\; \left(\frac{u+1}{u-1}\right)^{m/2} \left(\frac{1-u}{2}\right)^{m} {}_2F_1\left(m-\ell, \ell+m+1, m+1; \frac{1-u}{2}\right)\,. \tag{5.31b}$$

The ${}_2F_1$ function, which is sometimes simply denoted as F, is discussed in greater detail in the Handbook of Mathematical Functions edited by Milton Abramowitz and Irene A. Stegun, Publication AMS55 issued by the National Bureau of Standards (NBS).

Finally, we note that the relations (5.27) and (5.31), which, *a priori*, hold only for $|z| < 1$ and $|u| < 1$, respectively, can be extended beyond the circle of convergence of the respective series, by analytic continuation.

5.1.3 Spherical Harmonics

The Laplace and Poisson equations in spherical coordinates are encountered in a wide range of problems (electromagnetism, thermodynamics, mechanics of continuous media, and quantum mechanics). As might be expected, the solutions of these equations have been well studied. The solutions to the angular part of the equation are the spherical harmonics. These are the appropriately normalized products of the associated Legendre polynomials in $\cos\theta$ and the $\exp(\mathrm{i}m\varphi)$,

$$Y_{\ell m}(\theta,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}\,\frac{(\ell-m)!}{(\ell+m)!}}\,P_\ell^m(\cos(\theta))\;\mathrm{e}^{\mathrm{i}m\varphi}\,. \tag{5.32}$$

The $Y_{\ell m}(\theta,\varphi)$ are solutions to Eq. (5.12),

$$\vec{L}^2\,Y_{\ell m}(\theta,\varphi) = \ell\,(\ell+1)\,Y_{\ell m}(\theta,\varphi)\,, \tag{5.33}$$

and they have the property that

$$\vec{L}_z\,Y_{\ell m}(\theta,\varphi) = -\mathrm{i}\frac{\partial}{\partial\varphi}\,Y_{\ell m}(\theta,\varphi) = m\,Y_{\ell m}(\theta,\varphi)\,. \tag{5.34}$$

Other useful properties are given by

$$Y_{\ell\,-m}(\theta,\varphi) = (-1)^m\;Y_{\ell m}(\theta,\varphi)^*\;, \tag{5.35a}$$

$$Y_{\ell\,m}(\pi-\theta,2\pi-\varphi) = (-1)^\ell\;Y_{\ell\,-m}(\theta,\varphi)\;, \tag{5.35b}$$

$$Y_{\ell\,m}(\pi-\theta,\pi+\varphi) = (-1)^\ell\;Y_{\ell\,m}(\theta,\varphi)\;. \tag{5.35c}$$

The last one of these is the parity transformation. The orthonormality condition is

$$\int_0^{2\pi}\int_0^{\pi} Y^*_{\ell'\,m'}(\theta,\varphi)\;Y_{\ell m}(\theta,\varphi)\;\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi \;=\; \delta_{\ell\ell'}\,\delta_{mm'}\,, \tag{5.36a}$$

$$\langle Y_{\ell'm'}|\,Y_{\ell m}\rangle \;=\; \delta_{\ell\ell'}\,\delta_{mm'}\,, \tag{5.36b}$$

and the completeness condition reads

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y_{\ell\,m}(\theta,\varphi)\;Y^*_{\ell m}(\theta',\varphi') = \frac{1}{\sin\theta}\delta(\theta-\theta')\;\delta(\varphi-\varphi') = \delta(\varphi-\varphi')\;\delta(\cos\theta-\cos\theta')\;. \tag{5.36c}$$

For $\ell = 0$, the one existing spherical harmonic is only a constant,

$$Y_{00}(\theta,\varphi) = \left(\frac{1}{4\pi}\right)^{1/2}\,. \tag{5.37}$$

For $\ell = 1$, the spherical harmonics read as follows,

$$Y_{10}(\theta,\varphi) = \left(\frac{3}{4\pi}\right)^{1/2}\cos(\theta)\;, \tag{5.38a}$$

$$Y_{11}(\theta,\varphi) = -\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\;\mathrm{e}^{\mathrm{i}\varphi}\,,\qquad Y_{1\,-1}(\theta,\varphi) = \left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\;\mathrm{e}^{-\mathrm{i}\varphi}\;. \tag{5.38b}$$

The spherical harmonics with $\ell = 2$ are of second order in the trigonometric functions $\sin\theta$ and $\cos\theta$, and Y_{20} is proportional to $P_2(\cos\theta) = \frac{3}{2}\ \cos^2\theta - \frac{1}{2}$,

$$Y_{20}\,(\theta,\varphi) = \left(\frac{5}{4\pi}\right)^{1/2} \left[\frac{3}{2}\cos^2\theta - \frac{1}{2}\right]\,, \tag{5.39a}$$

$$Y_{21}\,(\theta,\varphi) = -\left(\frac{15}{8\pi}\right)^{1/2}\ \sin\theta\ \cos\theta\,\mathrm{e}^{\mathrm{i}\varphi}\,, \qquad Y_{2\,-1}\,(\theta,\varphi)\ =\ \left(\frac{15}{8\pi}\right)^{1/2}\ \sin\theta\ \cos\theta\,\mathrm{e}^{-\mathrm{i}\varphi}\,, \tag{5.39b}$$

$$Y_{22}\,(\theta,\varphi) = \left(\frac{15}{32\pi}\right)^{1/2}\ \sin^2\theta\,\mathrm{e}^{2\mathrm{i}\varphi}\,, \qquad Y_{2\,-2}\,(\theta,\varphi)\ =\ \left(\frac{15}{32\pi}\right)^{1/2}\ \sin^2\theta\,\mathrm{e}^{-2\mathrm{i}\varphi}\,. \tag{5.39c}$$

For $\ell = 3$, we have

$$Y_{30}\,(\theta,\varphi) = \left(\frac{7}{4\pi}\right)^{1/2}\ \left[\frac{5}{2}\cos^3\theta - \frac{3}{2}\cos\theta\right]\,, \tag{5.40a}$$

$$Y_{31}\,(\theta,\varphi) = -\left(\frac{21}{64\pi}\right)^{1/2}\ \sin\theta\left[5\cos^2\theta - 1\right]\ \mathrm{e}^{\mathrm{i}\varphi}\,, \quad Y_{3\,-1}\,(\theta,\varphi)\ =\ \left(\frac{21}{64\pi}\right)^{1/2}\ \sin\theta\left[5\cos^2\theta - 1\right]\ \mathrm{e}^{-\mathrm{i}\varphi}\,, \tag{5.40b}$$

$$Y_{32}\,(\theta,\varphi) = \left(\frac{105}{32\pi}\right)^{1/2}\ \sin^2\theta\ \cos\theta\,\mathrm{e}^{2\mathrm{i}\varphi}\,, \qquad Y_{3\,-2}\,(\theta,\varphi)\ =\ \left(\frac{105}{32\pi}\right)^{1/2}\ \sin^2\theta\ \cos\theta\,\mathrm{e}^{-2\mathrm{i}\varphi}\,, \tag{5.40c}$$

$$Y_{33}\,(\theta,\varphi) = -\left(\frac{35}{64\pi}\right)^{1/2}\ \sin^3\theta\,\mathrm{e}^{3\mathrm{i}\varphi}\,, \qquad Y_{3\,-3}\,(\theta,\varphi)\ =\ \left(\frac{35}{64\pi}\right)^{1/2}\ \sin^3\theta\,\mathrm{e}^{-3\mathrm{i}\varphi}\,. \tag{5.40d}$$

These functions are illustrated in Fig. 5.1.

5.1.4 Poisson Equation with a Point Charge in Spherical Coordinates

We will now re-examine the solution to the Poisson equation with a point charge q. Let the charge lie at coordinates (r',θ',φ') and let the observation point have coordinates (r,θ,φ). The solution will be a Green function and we consider the dependence on (r',θ',φ') and on (r,θ,φ). The charge density is

$$\begin{aligned}\rho(r,\theta,\varphi) &= q\ \delta(\vec{r}-\vec{r}')\\ &= \frac{q}{r'^{\,2}}\delta\left(r-r'\right)\ \delta\left(\cos\theta-\cos\theta'\right)\ \delta\left(\varphi-\varphi'\right) = q\ \delta^{(3)}(\vec{r}-\vec{r}')\,.\end{aligned} \tag{5.41}$$

and the Poisson equation for the "standard potential" $\Phi(\vec{r}) = \Phi(r,\theta,\varphi)$ reads as

$$\vec{\nabla}^2\ \Phi\left(r,\theta,\varphi\right) = -\frac{1}{\epsilon_0}\ \rho\left(r,\theta,\varphi\right) = -\frac{q}{\epsilon_0}\ \delta^{(3)}(\vec{r}-\vec{r}')\,. \tag{5.42}$$

Here, the subscript $\vec{r}'$ indicates the dependence on the position of the point charge. We have to keep both the position of the point charge at $\vec{r}'$ as well as the observation point $\vec{r}$ as variables.

For the remainder of the current section, we shall use $\Phi\left(r,\theta,\varphi\right)$ in terms of the "standard potential" which fulfills Eq. (5.42) and depends, strictly speaking, both on the observation point $\vec{r}$ as well as the point $\vec{r}'$

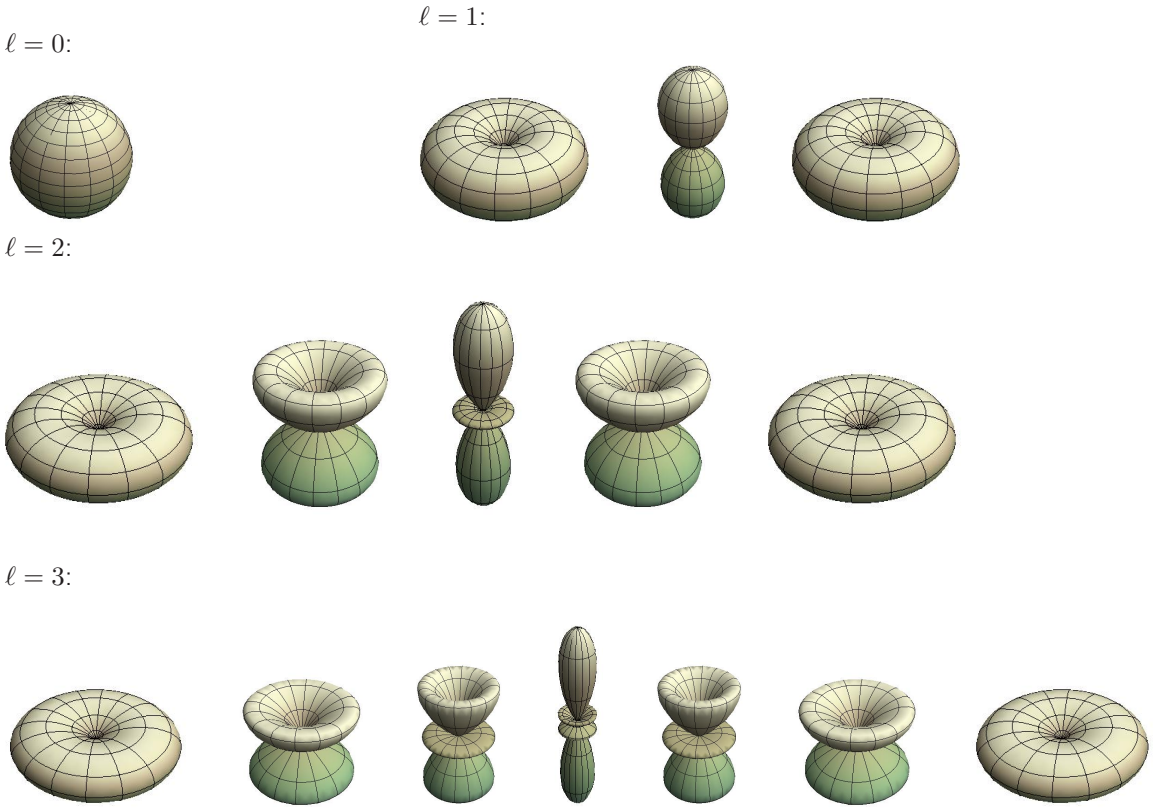

Figure 5.1: We illustrate the shape of the spherical harmonic functions $Y_{\ell m}(\theta, \varphi)$ for $\ell = 0, 1, 2, 3$ by plotting $f(\theta, \varphi) = |Y_{\ell m}(\theta, \varphi)|^2$ as a function of the polar angle θ and of the azimuth angle φ, i.e., we plot the set of points $f(\theta, \varphi)\,(\hat{\mathrm{e}}_x \sin\theta \cos\varphi + \hat{\mathrm{e}}_y \sin\theta \sin\varphi + \hat{\mathrm{e}}_z \cos\theta)$. The sequence of magnetic components is from $m = -\ell$ to $m = \ell$.

where the point charge is located. This ansatz is matched against the Green function as follows,

$$\Phi\left(\vec{r}\right) = \Phi\left(r, \theta, \varphi\right) = -\frac{q}{\epsilon_0}\, g(\vec{r}, \vec{r}')\,, \qquad \vec{\nabla}^2\, g(\vec{r}, \vec{r}') = \delta^{(3)}(\vec{r} - \vec{r}')\,. \tag{5.43}$$

Ansatz for the Green Function. We look for a solution of the form

$$\Phi\left(r, \theta, \varphi\right) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} f_{\ell m}\left(r; r', \theta', \varphi'\right)\; Y_{\ell m}\left(\theta, \varphi\right)\,. \tag{5.44}$$

Inserting this into the Poisson equation, we obtain

$$\vec{\nabla}^2 \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} f_{\ell m}\left(r; r', \theta', \varphi'\right)\; Y_{\ell m}\left(\theta, \varphi\right) = -\frac{q}{\epsilon_0\; r'^{\,2}}\; \delta\left(r - r'\right)\; \delta\left(\cos\theta - \cos\theta'\right)\; \delta\left(\varphi - \varphi'\right)\,. \tag{5.45}$$

After the separation of angular and radial variables, this equation becomes

$$\frac{1}{r^2}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\left[\left(\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}-\ell\left(\ell+1\right)\right)f_{\ell m}(r;r',\theta',\varphi')\right]Y_{\ell m}\left(\theta,\varphi\right)$$

$$=-\frac{q}{\epsilon_0\,r^2}\,\delta\left(r-r'\right)\,\delta\left(\cos\theta-\cos\theta'\right)\,\delta\left(\varphi-\varphi'\right)\,. \tag{5.46}$$

In the prefactor, we could have replaced r by r', because of the Dirac-δ. We multiply both sides by $Y^*_{\ell' m'}\left(\theta,\varphi\right)$, and integrate over

$$\int \mathrm{d}\Omega=\int_{-1}^{1}\mathrm{d}(\cos\theta)\int_0^{2\pi}\mathrm{d}\varphi=\int_0^{\pi}\mathrm{d}\theta\,\sin\theta\int_0^{2\pi}\mathrm{d}\varphi\,. \tag{5.47}$$

Using the orthonormality of the spherical harmonics, we find that

$$\frac{1}{r^2}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\left[\left(\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}-\ell\left(\ell+1\right)\right)f_{\ell m}(r;r',\theta',\varphi')\right]\,\delta_{\ell'\,\ell}\,\delta_{m'\,m}$$

$$=-\frac{q}{\epsilon_0\,r'^2}\,\delta\left(r-r'\right)\int_{-1}^{1}\mathrm{d}(\cos\theta)\,\int_0^{\pi}\mathrm{d}\varphi\,\delta\left(\varphi-\varphi'\right)\delta\left(\cos\theta-\cos\theta'\right)Y^*_{\ell' m'}\left(\theta,\varphi\right)\,, \tag{5.48}$$

where we use the operator identity

$$\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}=\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\,. \tag{5.49}$$

After the θ and φ integrations, we obtain

$$\frac{1}{r^2}\,\left[\left(\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}-\ell'\,\left(\ell'+1\right)\right)f_{\ell' m'}(r;r',\theta',\varphi')\right]=-\frac{q}{\epsilon_0\,r'^2}\,\delta\left(r-r'\right)\,Y^*_{\ell' m'}\left(\theta',\varphi'\right)\,. \tag{5.50}$$

Thus, the angular dependence of $f_{\ell m}\left(r;r',\theta',\varphi'\right)$ is given by $Y^*_{\ell m}\left(\theta',\varphi'\right)$. We now redefine $\ell'\to\ell$ and $m'\to m$ and write

$$f_{\ell m}\left(r;r',\theta',\varphi'\right)=g_\ell\left(r;r'\right)\,Y^*_{\ell m}\left(\theta',\varphi'\right)\,. \tag{5.51}$$

Radial Equation. The functions $g_\ell\left(r;r'\right)$ thus satisfy

$$\frac{1}{r^2}\left[\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}-\ell\left(\ell+1\right)\right]\,g_\ell\left(r,r'\right)=-\frac{q}{\epsilon_0\,r^2}\,\delta\left(r-r'\right)\,. \tag{5.52}$$

We can also include the following, qualitative consideration: Namely, the radial Green function $g_\ell\left(r,r'\right)$ changes its functional form at the cusp $r=r'$. It has a "continuous kink". The first derivative with respect to r generates a true discontinuity, whereas the second derivative generates the Dirac-δ function required to match the right-hand side of Eq. (5.52).

Projection onto the Homogeneous Equation. This equation for the radial function is solved by the following method. We obtain the solutions to the homogeneous equations for $r<r'$ and $r>r'$. We then make $g_\ell\left(r;r'\right)$ continuous at $r=r'$, and satisfy the condition placed on $g_\ell\left(r;r'\right)$ obtained by integrating Eq. (5.52) from $r=r'-\varepsilon$ to $r=r'+\varepsilon$. The solution to the homogeneous equation in r has the general form

$$g_\ell\left(r;r'\right)=\alpha_\ell\,\left(r'\right)r^\ell+\beta_\ell\left(r'\right)r^{-\ell-1}\,. \tag{5.53}$$

For $r < r'$, we have $g_\ell(r;r') = \alpha_\ell(r')\, r^\ell$, and for $r > r'$, we have $g_\ell(r;r') = \beta_\ell(r')\, r^{-\ell-1}$. Continuity at $r = r'$ requires that

$$g_\ell(r;r') = a_\ell \frac{r^\ell}{r'^{\,\ell+1}}, \qquad r < r', \tag{5.54a}$$

$$g_\ell(r;r') = a_\ell \frac{r'^{\,\ell}}{r^{\ell+1}}, \qquad r > r', \tag{5.54b}$$

so that $g_\ell(r;r') = c\, f_{\mathrm{reg}=0}(r_<)\, f_{\mathrm{reg}=\infty}(r_>)$.

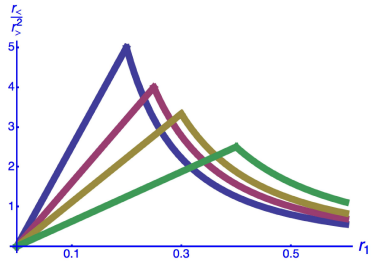

Figure 5.2: Plot of the function $f(r_1, r_2) = r_</r_>^2$ as a function of r_1 for $r_2 = 0.2, 0.25, 0.3$ and 0.4. The maximum is reached at $r_1 = r_2$, with $f(r_1, r_1) = 1/r_1$. This implies that for $r_2 = 0.2$, the maximum (kink) is at $f = 5$.

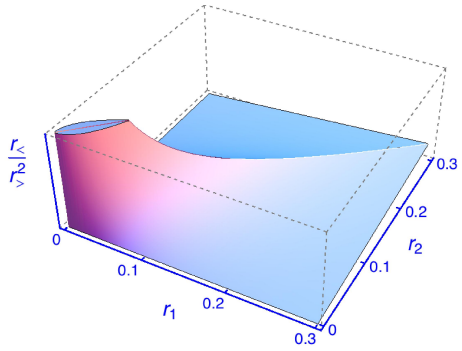

Figure 5.3: Three-dimensional plot of the function $f(r_1, r_2) = r_</r_>^2$ which occurs in the dipole term $\ell = 1$ of Eq. (5.75).

Integrating Eq. (5.52) from $r = r' - \varepsilon$ to $r = r' + \varepsilon$, we obtain

$$\int_{r'-\varepsilon}^{r'+\varepsilon} \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} g_\ell\right) - \ell(\ell+1)\, g_\ell\right] \mathrm{d}r = -\frac{q}{\epsilon_0} \int_{r'-\varepsilon}^{r'+\varepsilon} \frac{1}{r^2}\, \delta(r - r')\, \mathrm{d}r\,. \tag{5.55}$$

The second term on the left is continuous at $r = r'$ and drops out of the equation, and so

$$\int_{r'-\varepsilon}^{r'+\varepsilon} \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} g_\ell\right) \mathrm{d}r = -\frac{q}{\epsilon_0 r'^2}\,. \tag{5.56}$$

Integrating by parts once, we finally obtain

$$\frac{1}{r^2}\left(r^2 \frac{\partial}{\partial r} g_\ell(r;r')\right)\Big|_{r=r'-\varepsilon}^{r=r'+\varepsilon} + \int_{r'-\varepsilon}^{r'+\varepsilon} \frac{2}{r}\left(\frac{\partial}{\partial r} g_\ell(r;r')\right)\, \mathrm{d}r = -\frac{q}{\epsilon_0\, r'^{\,2}}\,. \tag{5.57}$$

After an additional integration by parts, we obtain

$$\frac{1}{r^2}\left(r^2\frac{\partial}{\partial r}g_\ell(r;r')\right)\Big|_{r=r'-\varepsilon}^{r=r'+\varepsilon}+\frac{2}{r}\,g_\ell(r;r')\Big|_{r=r'-\varepsilon}^{r=r'+\varepsilon}+\int_{r'-\varepsilon}^{r'+\varepsilon}\frac{2}{r^2}\,g_\ell(r;r')\,\mathrm{d}r=-\frac{q}{\epsilon_0\,r'^2}\,. \tag{5.58}$$

Only the first term on the left is non-zero at $r=r'$, and so

$$\lim_{\epsilon\to 0}\left\{r'^2\,\left[\left(\frac{\partial g_\ell\,(r;r')}{\partial r}\right)_{r=r'+\varepsilon}-\left(\frac{\partial g_\ell\,(r;r')}{\partial r}\right)_{r=r'-\varepsilon}\right]\right\}=-\frac{q}{\epsilon_0}\,. \tag{5.59}$$

We now use the specific forms for $g_\ell\,(r;r')$ and obtain

$$r'^2\,a_\ell\,\left[\left(\frac{\partial}{\partial r}\frac{r'^\ell}{r^{\ell+1}}\right)_{r=r'}-\left(\frac{\partial}{\partial r}\frac{r^\ell}{r'^{\ell+1}}\right)_{r=r'}\right]=-\frac{q}{\epsilon_0}\,, \tag{5.60}$$

which can be reformulated as follows (we pull out the non-differentiated variable as a prefactor)

$$r'^2\,a_\ell\,\left[r'^\ell\left(\frac{\partial}{\partial r}\frac{1}{r^{\ell+1}}\right)_{r=r'}-\frac{1}{r'^{\ell+1}}\left(\frac{\partial}{\partial r}r^\ell\right)_{r=r'}\right]=-\frac{q}{\epsilon_0}\,, \tag{5.61}$$

and

$$r'^{\,2}\,a_\ell\,\left[-(\ell+1)\frac{r'^\ell}{r'^{\ell+2}}-\ell\frac{r'^{\ell-1}}{r'^{\,\ell+1}}\right]=a_\ell\,\left\{-(\ell+1)-\ell\right\}=-a_\ell\,(2\ell+1)=-\frac{q}{\epsilon_0}\,. \tag{5.62}$$

Thus, we obtain the prefactor in Eq. (5.54a) as

$$a_\ell=\frac{q}{\epsilon_0\,(2\ell+1)}\,. \tag{5.63}$$

An alternative, easier derivation is as follows. Let us start again from Eq. (5.56),

$$\int_{r'-\varepsilon}^{r'+\varepsilon}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}g_\ell\right)\mathrm{d}r=-\frac{q}{\epsilon_0 r'^2}\,,\qquad\int_{r'-\varepsilon}^{r'+\varepsilon}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}g_\ell\right)\mathrm{d}r=-\frac{q}{\epsilon_0}\,. \tag{5.64}$$

The prefactor assumes the value $1/r^2\approx 1/r'^2$, but the derivative of g_ℓ may have a jump. Hence,

$$\left[\left(r^2\frac{\partial}{\partial r}g_\ell\right)\right]_{r=r'-\epsilon}^{r=r'+\epsilon}=-\frac{q}{\epsilon_0}\,, \tag{5.65}$$

or

$$\left[\left(\frac{\partial}{\partial r}g_\ell\right)\right]_{r=r'-\epsilon}^{r=r'+\epsilon}=-\frac{q}{\epsilon_0\,r'^2}\,, \tag{5.66}$$

Using

$$g_\ell\,(r;r')=a_\ell\,\frac{r_<^\ell}{r_>^{\ell+1}} \tag{5.67}$$

one obtains

$$-\frac{a_\ell\,(-\ell-1)\,r'^\ell}{r'^{\ell+2}}-a_\ell\frac{\ell r'^{\ell-1}}{r'^{\ell+1}}=-\frac{2\ell+1}{r'^2}\,a_\ell=-\frac{q}{\epsilon_0\,r'^2}\,. \tag{5.68}$$

So,

$$a_\ell=\frac{q}{\epsilon_0\,(2\ell+1)}\,. \tag{5.69}$$

Let us collect all prefactors. According to Eq. (5.42), we were looking for the solution of the equation

$$\vec{\nabla}^2\,\Phi\,(r,\theta,\varphi) = -\frac{1}{\epsilon_0}\,\rho\,(r,\theta,\varphi) = -\frac{1}{\epsilon_0}\,q\,\delta^{(3)}\,(\vec{r},\vec{r}')\;. \tag{5.70}$$

On the basis of Eqs. (5.44) and (5.51), we can write the solution as

$$\Phi\,(r,\theta,\varphi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} g_\ell\,(r;r')\;Y_{\ell m}\,(\theta,\varphi)\;Y^*_{\ell m}\,(\theta',\varphi')\;. \tag{5.71}$$

Finally, Eqs. (5.54a) and (5.54b) together with Eq. (5.63) can be summarized as follows,

$$g_\ell\,(r;r') = a_\ell\,\frac{r_<^\ell}{r_>^{\ell+1}} = \frac{q}{\epsilon_0\,(2\ell+1)}\,\frac{r_<^\ell}{r_>^{\ell+1}}\,,\qquad r_< = \min(r;r')\,,\qquad r_> = \max(r;r')\,. \tag{5.72}$$

Putting everything together, we have

$$\Phi\,(r,\theta,\varphi) = \frac{q}{\epsilon_0}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{1}{2\ell+1}\,\frac{r_<^\ell}{r_>^{\ell+1}}\,Y_{\ell m}\,(\theta,\varphi)\;Y^*_{\ell m}\,(\theta',\varphi')\;. \tag{5.73}$$

On the other hand, we can write down the solution of $\Phi\,(r,\theta,\varphi)$ immediately,

$$\Phi\,(r,\theta,\varphi) = \frac{1}{4\pi\epsilon_0}\,\frac{q}{|\vec{r}-\vec{r}'|}\;. \tag{5.74}$$

Multipole Expansion. We can thus also write the following equation,

Multipole Expansion:

$$\frac{1}{|\vec{r}-\vec{r}'|} = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{4\pi}{2\ell+1}\,\frac{r_<^\ell}{r_>^{\ell+1}}\,Y_{\ell m}\,(\theta,\varphi)\;Y^*_{\ell m}\,(\theta',\varphi')\;, \tag{5.75}$$

which is the basis for all so called multipole expansions in electrodynamics, and thus very important. The case-by-case differentiation according to $r_<$ and $r_>$ for $\ell = 1$ is illustrated in Figs. 5.2 and 5.3.

5.1.5 Green Function and Expansion of $1/|\vec{r}-\vec{r}'|$

In view of the above, the Green function of electrostatics can be formulated as

$$g(\vec{r},\vec{r}') = -\frac{1}{4\pi\,|\vec{r}-\vec{r}'|} = -\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{1}{2\ell+1}\,\frac{r_<^\ell}{r_>^{\ell+1}}\,Y_{\ell m}\,(\theta,\varphi)\;Y^*_{\ell m}\,(\theta',\varphi') \tag{5.76}$$

which satisfies (we recall):

$$\vec{\nabla}^2\;g(\vec{r},\vec{r}') = \delta(\vec{r}-\vec{r}')\,. \tag{5.77}$$

This function provides a convenient way to evaluate integrals of the form

$$\Phi(\vec{r}) = -\frac{1}{\epsilon_0}\int g(\vec{r},\vec{r}')\;\rho(\vec{r}')\;\mathrm{d}^3r' \tag{5.78}$$

for extended charge distributions $\rho(\vec{r}')$.

Example. We determine the electrostatic potential due to the following distribution of charge (a spherical shell of charge with a $\cos\theta$ angular dependence),

$$\rho(\vec{r}) = \frac{Q}{a^2}\;\cos\theta\;\delta(r-a)\,, \tag{5.79}$$

and the potential is to be determined under the assumption that it goes to zero at least as fast as $1/r$ in the limit $r \to \infty$.

Solution. Conceivable surface integrals at infinity vanish. So, we calculate

$$\Phi(\vec{r}) = -\frac{1}{\epsilon_0}\int_{\mathbb{R}^3} g(\vec{r},\vec{r}')\,\rho(\vec{r}')\,\mathrm{d}^3r' = +\frac{1}{\epsilon_0}\int_{\mathbb{R}^3}\frac{1}{4\pi}\,\frac{1}{|\vec{r}-\vec{r}'|}\,\rho(\vec{r}')\,\mathrm{d}^3r' \tag{5.80}$$

$$= \frac{1}{4\pi\epsilon_0}\int_{\mathbb{R}^3}\frac{Q}{a^2}\cos\theta'\,\delta(r'-a)\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{4\pi}{2\ell+1}\frac{r_<^\ell}{r_>^{\ell+1}}\,Y_{\ell m}(\theta,\varphi)\;Y^*_{\ell m}(\theta',\varphi')\,\mathrm{d}^3r'$$

$$= \frac{1}{4\pi\epsilon_0}\,\frac{Q}{a^2}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{4\pi}{2\ell+1}Y_{\ell m}(\theta,\varphi)\int_0^\infty\frac{r_<^\ell}{r_>^{\ell+1}}\,r'^2\,\delta(r'-a)\,\mathrm{d}r'\int\cos\theta'\,Y^*_{\ell m}(\theta',\varphi')\;\mathrm{d}(\cos\theta')\mathrm{d}\varphi'\,.$$

The situation now is as follows. If we can identify the angular dependence given by the function $\cos\theta'$ as a combination of spherical harmonics, then it is possible to use the orthonormality and completeness relations (5.36) and carry out the angular integrations without problems. Indeed, this is possible. We identify $\cos\theta'$ as a spherical harmonic,

$$\cos\theta' = \sqrt{\frac{4\pi}{3}}\,Y_{10}(\theta',\varphi')\,. \tag{5.81}$$

We can thus write

$$\Phi(\vec{r}) = \frac{1}{4\pi\epsilon_0}\,\frac{Q}{a^2}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{4\pi}{2\ell+1}\,Y_{\ell m}(\theta,\varphi)\int_0^\infty\frac{r_<^\ell}{r_>^{\ell+1}}\,r'^2\,\delta(r'-a)\,\mathrm{d}r'\sqrt{\frac{4\pi}{3}}\,\langle Y_{\ell m}|\,Y_{10}\rangle$$

$$= \frac{1}{4\pi\epsilon_0}\,\frac{Q}{a^2}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{4\pi}{2\ell+1}\,Y_{\ell m}(\theta,\varphi)\int_0^\infty\frac{r_<^\ell}{r_>^{\ell+1}}\,r'^2\,\delta(r'-a)\,\mathrm{d}r'\,\sqrt{\frac{4\pi}{3}}\delta_{\ell 1}\delta_{m0}$$

$$= \frac{1}{\epsilon_0}\frac{Q}{a^2}\frac{1}{2\cdot 1+1}\,\sqrt{\frac{4\pi}{3}}\,Y_{10}(\theta,\varphi)\int_0^\infty\frac{r_<}{r_>^2}\,r'^2\,\delta(r'-a)\,\mathrm{d}r'$$

$$= \frac{1}{\epsilon_0}\frac{Q}{3a^2}\,\sqrt{\frac{4\pi}{3}}\,Y_{10}(\theta,\varphi)\int_0^\infty\frac{\min(r,r')}{\max(r,r')^2}\,r'^2\,\delta(r'-a)\,\mathrm{d}r'$$

$$= \frac{Q}{3\,\epsilon_0\,a^2}\,\cos\theta\,\frac{\min(a,r)}{\max(a,r)^2}\,a^2$$

$$= \begin{cases}\dfrac{Q}{3\epsilon_0}\,\dfrac{r}{a^2}\,\cos\theta\,, & r<a\\[2ex] \dfrac{Q}{3\epsilon_0}\,\dfrac{a}{r^2}\,\cos\theta\,, & r>a\,.\end{cases} \tag{5.82}$$

Continuity at $r=a$ is thus preserved.

5.1.6 Multipole Expansion of Charge Distributions

General Multipole Expansion. We now come to what is perhaps the most important aspect of electrostatics taught in this course. We recall that

$$g(\vec{r},\vec{r}') = -\frac{1}{4\pi\,|\vec{r}-\vec{r}'|} = -\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{1}{2\ell+1}\,\frac{r_<^{\ell}}{r_>^{\ell+1}}\,Y_{\ell m}\,(\theta,\varphi)\;Y_{\ell m}^{*}\,(\theta',\varphi')\;, \tag{5.83}$$

and that

$$\Phi(\vec{r}) = -\frac{1}{\epsilon_0}\int g(\vec{r},\vec{r}')\;\rho(\vec{r}')\;\mathrm{d}^3r'\,, \tag{5.84}$$

for extended charge distributions $\rho(\vec{r}')$. So, if the charge distribution is localized and we calculate the potential outside of the localized distribution ($r > r'$), then

Multipole Moment Decomposition:

$$\Phi\,(\vec{r}) = \frac{1}{\epsilon_0}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{1}{2\ell+1}\,\frac{Y_{\ell m}\,(\theta,\varphi)}{r^{\ell+1}}\,\left(\int\rho\,(\vec{r}')\;r'^{\,\ell}\;Y_{\ell m}^{*}\,(\theta',\varphi')\;\mathrm{d}^3r'\right). \tag{5.85}$$

The integral in this expression defines the *multipole moments* of the charge distribution,

Multipole Moments:

$$q_{\ell m} = \int\rho\,(\vec{r})\;r^{\ell}\;Y_{\ell m}^{*}\,(\theta,\varphi)\;\mathrm{d}^3r\,. \tag{5.86}$$

Furthermore, because of the relationship $Y_{\ell\,-m}\,(\theta,\varphi) = (-1)^m\;Y_{\ell m}^{*}\,(\theta,\varphi)$, it follows that

$$q_{\ell\,-m} = (-1)^m\;q_{\ell m}^{*}\,. \tag{5.87}$$

Potential in Terms of Multipole Moments. In terms of the multipole moments of the charge distribution, the potential for $r > R$ is

Multipole Expansion:

$$\Phi\,(\vec{r}) = \frac{1}{\epsilon_0}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{q_{\ell m}}{2\ell+1}\,\frac{Y_{\ell m}\,(\theta,\varphi)}{r^{\ell+1}}\,. \tag{5.88}$$

The set of elements $\{q_{\ell\,m};\,m=-\ell,\;-\ell+1,\;\ldots,\;\ell-1,\;\ell\}$ form a spherical tensor of rank ℓ. There are two common representations of tensors, the familiar rectilinear representation (in Cartesian coordinates) and the spherical representation.

5.1.7 Dipole Term in Cartesian and Spherical Coordinates

The multipole decomposition, in Cartesian coordinates, is based on the expansion

$$\frac{1}{|\vec{r}-\vec{r}'|} = \frac{1}{r} + \frac{\vec{r}\cdot\vec{r}'}{r^3} + \frac{3(\vec{r}\cdot\vec{r}')^2 - r^2\,r'^2}{2r^5} + \mathcal{O}(r^{-4})\,. \tag{5.89}$$

This leads to the following expansion for the potential,

$$\begin{aligned}\Phi(\vec{r}) &= \frac{1}{4\pi\epsilon_0}\int\mathrm{d}^3r'\,\frac{1}{|\vec{r}-\vec{r}'|}\,\rho(\vec{r}')\\ &\approx \frac{1}{4\pi\epsilon_0}\int\mathrm{d}^3r'\,\left(\frac{1}{r}+\frac{\vec{r}\cdot\vec{r}'}{r^3}+\frac{3(\vec{r}\cdot\vec{r}')^2-r^2\,r'^2}{2r^5}\right)\rho(\vec{r}')\\ &\approx \frac{Q}{4\pi\epsilon_0\,r}+\frac{\vec{r}\cdot\vec{p}}{4\pi\epsilon_0\,r^3}+\frac{1}{4\pi\epsilon_0}\,\frac{Q_{ij}\,(3r_i\,r_j-\delta_{ij}\,r^2)}{2r^5}+\ldots\,,\end{aligned} \tag{5.90}$$

where the total charge Q, the dipole moment vector $\vec{p}$, and the components of the quadrupole tensor Q_{ij} are given as

$$Q = \int \mathrm{d}^3 r' \, \rho(\vec{r}') \,, \tag{5.91a}$$

$$\vec{p} = \int \mathrm{d}^3 r' \, \vec{r}' \, \rho(\vec{r}') \,, \tag{5.91b}$$

$$Q_{ij} = \int \mathrm{d}^3 r' \, \left(3 r'_i \, r'_j - \delta_{ij} \, \vec{r}^{\,\prime\, 2} \right) \, \rho(\vec{r}') \,. \tag{5.91c}$$

Let us focus on the dipole term, which is given by the term with $\ell = 1$ in Eq. (5.85),

$$\Phi\left(\vec{r}\right)|_{\ell=1} \sim \frac{1}{\epsilon_0} \, \sum_{m=-1}^{1} \frac{1}{3} \, \frac{Y_{\ell m}\left(\theta, \varphi\right)}{r^2} \, \left(\int \mathrm{d}^3 r' \, r' \, \rho\left(\vec{r}'\right) \, Y^*_{\ell m}\left(\theta', \varphi'\right) \right) \,. \tag{5.92}$$

We now anticipate the addition theorem of spherical harmonics, given in Eq. (5.121) below,

$$P_\ell\left(\cos \angle(\vec{r}, \vec{r}')\right) = \frac{4\pi}{2\ell + 1} \, \sum_{m=-\ell}^{\ell} Y_{\ell m}\left(\theta, \varphi\right) \, Y^*_{\ell m}\left(\theta', \varphi'\right) \,, \tag{5.93}$$

so that for $\ell = 1$,

$$P_1\left(\cos \angle(\vec{r}, \vec{r}')\right) = \hat{r} \cdot \hat{r}' = \frac{4\pi}{3} \, \sum_{m=-1}^{1} Y_{1m}\left(\theta, \varphi\right) \, Y^*_{1m}\left(\theta', \varphi'\right) \,. \tag{5.94}$$

Inserting this relationship into Eq. (5.92), one obtains

$$\begin{aligned} \Phi\left(\vec{r}\right)|_{\ell=1} &\sim \frac{1}{3 \, \epsilon_0 \, r^2} \, \left(\int \mathrm{d}^3 r' \, \frac{3}{4\pi} \, \hat{r} \cdot \hat{r}' \, r' \, \rho\left(\vec{r}'\right) \right) \\ &\sim \frac{1}{4\pi\epsilon_0} \, \frac{1}{r^3} \, \left(\int \mathrm{d}^3 r' \, \vec{r} \cdot \vec{r}' \, \rho\left(\vec{r}'\right) \right) = \frac{\vec{r} \cdot \vec{p}}{4\pi\epsilon_0 \, r^3} \,. \end{aligned} \tag{5.95}$$

It remains to clarify the relation of the components of the dipole moment vector, in the Cartesian versus the spherical representation. Indeed, in the spherical representation, we find that

$$q_{1\pm1} = \mp \sqrt{\frac{3}{8\pi}} \, \left(p_1 \mp \mathrm{i} \, p_2 \right) \,, \qquad q_{10} = \sqrt{\frac{3}{4\pi}} \, p_3 \,. \tag{5.96}$$

We can repeat the above calculation for the charge distribution in the formalism of the multipole moments. Let us remember that we considered the problem of a charge distribution

$$\rho(\vec{r}') = \frac{Q}{a^2} \, \cos\theta' \, \delta(r' - a) \,, \tag{5.97}$$

where we identified

$$\cos\theta' = \sqrt{\frac{4\pi}{3}} \, Y_{10}(\theta', \varphi') \,. \tag{5.98}$$

So,

$$
\begin{aligned}
q_{10} &= \int \rho\,(\vec{r}^{\,\prime})\ r'^{\,(\ell=1)}\ Y_{10}^{*}\,(\theta',\varphi')\ \mathrm{d}^3 r' \\
&= \int \rho\,(\vec{r}^{\,\prime})\ r'\ Y_{10}^{*}\,(\theta',\varphi')\ r'^2\,\mathrm{d}r'\,\mathrm{d}\Omega' \\
&= \sqrt{\frac{4\pi}{3}}\ \left(\int \frac{Q}{a^2}\,\delta(r'-a)\,r'^{2+1}\,\mathrm{d}r'\right)\left(\int Y_{10}(\theta',\varphi')\,Y_{10}^{*}\,(\theta',\varphi')\ \mathrm{d}\Omega'\right) \\
&= \sqrt{\frac{4\pi}{3}}\ \left(\int \frac{Q}{a^2}\,\delta(r'-a)\,r'^{3}\,\mathrm{d}r'\right)\left(\int Y_{10}(\theta',\varphi')\,Y_{10}^{*}\,(\theta',\varphi')\ \mathrm{d}\Omega'\right) \\
&= \sqrt{\frac{4\pi}{3}}\ Q\,a\,,
\end{aligned}
\tag{5.99}
$$

which has the correct physical dimension (charge $\times$ length) of a dipole moment. In terms of the multipole moments of the charge distribution, the potential for $r > R$ is finally found to be

$$
\Phi\,(\vec{r}) = \frac{1}{\epsilon_0}\ \sum_{\ell=0}^{\infty}\ \sum_{m=-\ell}^{\ell}\ \frac{q_{\ell m}}{2\ell+1}\ \frac{Y_{\ell m}\,(\theta,\varphi)}{r^{\ell+1}} = \frac{1}{\epsilon_0}\ \frac{q_{10}}{3}\ \frac{Y_{10}\,(\theta,\varphi)}{r^2} = \frac{q_{10}}{3\epsilon_0 r^2}\ \sqrt{\frac{3}{4\pi}}\ \cos\theta\,. \tag{5.100}
$$

We thus recover the result from Eq. (5.82) for the dipole potential,

$$
\Phi(\vec{r}) = \frac{Q\,a}{3\epsilon_0 r^2}\ \cos\theta\,, \tag{5.101}
$$

outside of the charge distribution. Other examples for charge distributions are given in Fig. 5.4.

The quadrupole term, by contrast, is given by the term with $\ell = 2$ in Eq. (5.85),

$$
\Phi\,(\vec{r})|_{\ell=2} \sim \frac{1}{\epsilon_0}\ \sum_{m=-2}^{2}\ \frac{1}{5}\ \frac{Y_{2m}\,(\theta,\varphi)}{r^3}\ \left(\int \mathrm{d}^3 r'\ r'^2\ \rho\,(\vec{r}^{\,\prime})\ Y_{2m}^{*}\,(\theta',\varphi')\right). \tag{5.102}
$$

The addition theorem implies that

$$
P_2\,(\cos\angle(\vec{r},\vec{r}^{\,\prime})) = \frac{1}{2}\ \left[3(\hat{r}\cdot\hat{r}')^2 - 1\right] = \frac{4\pi}{5}\ \sum_{m=-2}^{2}\ Y_{2m}\,(\theta,\varphi)\ Y_{2m}^{*}\,(\theta',\varphi')\ . \tag{5.103}
$$

Inserting this relationship into Eq. (5.102), one obtains

$$
\begin{aligned}
\Phi\,(\vec{r})|_{\ell=2} &\sim \frac{1}{\epsilon_0}\ \frac{1}{5}\ \left(\int \mathrm{d}^3 r'\ r'^2\ \rho\,(\vec{r}^{\,\prime})\ \frac{5}{4\pi}\ \frac{1}{2}\ \left[3(\hat{r}\cdot\hat{r}')^2 - 1\right]\right) \\
&= \frac{1}{4\pi\epsilon_0}\ \frac{1}{2r^5}\ \left(\int \mathrm{d}^3 r'\ r'^2\ \rho\,(\vec{r}^{\,\prime})\ \left(3(\vec{r}\cdot\vec{r}^{\,\prime})^2 - \vec{r}^{\,2}\ \vec{r}^{\,\prime 2}\right)\right) = \frac{1}{4\pi\epsilon_0}\ \frac{Q_{ij}(3r_i\,r_j - \delta_{ij}\,\vec{r}^{\,2})}{2r^5}\,.
\end{aligned}
\tag{5.104}
$$

Let us count. We have five components of the quadrupole tensor q_{2m} with $m = -2,\ldots,2$. The quadrupole tensor in Cartesian coordinates has the form

$$
(Q_{ij}) = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{32} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{12} & Q_{22} & Q_{32} \\ Q_{13} & Q_{23} & -Q_{11} - Q_{22} \end{pmatrix}, \tag{5.105}
$$

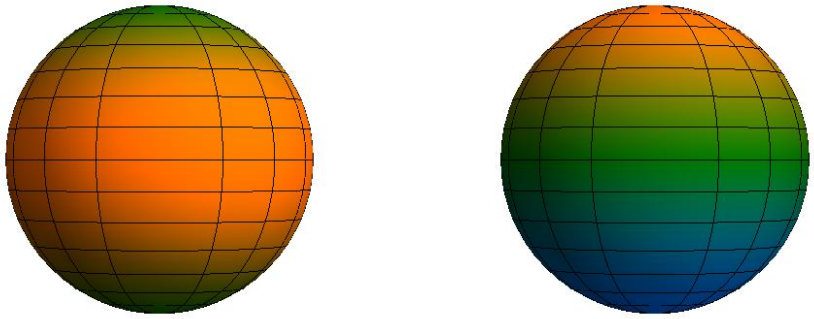

Figure 5.4: The left plot shows a sphere with a charge distribution $\rho(\vec{r}') = \dfrac{Q}{a^2}\ \sin\theta'\ \delta(r'-a)$, proportional to $\sin\theta'$. Red areas mark positive charge, and neutral areas are green. The right plot displays a sphere with a charge distribution $\rho(\vec{r}') = \dfrac{Q}{a^2}\ \cos\theta'\ \delta(r'-a)$. Blue areas denote negative charge. The plot on the right is a dipole charge distribution.

where we have used the symmetry $Q_{ij} = Q_{ji}$ and the tracelessness of the quadrupole tensor $\sum_{i=1}^{3} Q_{ii} = 0$ which holds in view of $\sum_{i=1}^{3} \delta_{ii} = 3$. Thus, because the quadrupole moment of the charge distribution is a symmetric, traceless second rank tensor, it is therefore specified by five parameters, as the second form in Eq. (5.105) suggests.

The simplest relationship occurs for q_{20} and Q_{33}. This simplicity is obtained because the spherical tensors we are using have taken the z or 3 axis as a preferred axis. We calculate:

$$\begin{aligned} Q_{33} &= \int \left(3\ z^2 - r^2\right)\ \rho\,(\vec{r})\ \mathrm{d}^3 r = \int \left(3\ \cos^2\theta - 1\right)\ r^2\ \rho\,(\vec{r})\ \mathrm{d}^3 r \\ &= \sqrt{\frac{16\pi}{5}} \int \sqrt{\frac{5}{16\pi}}\ \left(3\ \cos^2\theta - 1\right)\ r^2\ \rho\,(\vec{r})\ \mathrm{d}^3 r \\ &= 4\sqrt{\frac{\pi}{5}} \int Y_{20}(\theta,\varphi)\ r^2\ \rho\,(\vec{r})\ \mathrm{d}^3 r = 4\sqrt{\frac{\pi}{5}}\ q_{20}\,. \end{aligned} \tag{5.106}$$

5.1.8 Multipole Expansion in an External Field

Up to now, we have considered the multipole decomposition in spherical coordinates, and we have considered the original charge distribution to be centered about the point $\vec{r}' \approx 0$, with a distant observation point $\vec{r}$. An expansion of $1/|\vec{r} - \vec{r}'|$ into multipoles (spherical coordinates) then leads to the multipole decomposition. The total charge of the charge distribution that generates the potential at $\vec{r}$ is the monopole.

In order to switch the formalism of the multipole decomposition to Cartesian coordinates, we consider an opposite situation, in some sense. A charge distribution is centered about the point $\vec{r} = \vec{0}$, with the potential being generated by a distant charge distribution that is centered about the point $\vec{r}' \neq \vec{0}$. The distant charge distribution generates a potential $\Phi(\vec{r})$ which interacts with the charge distribution $\rho(\vec{r})$. The potential energy

of the configuration is given by the overlap integral

$$W = \int \rho\,(\vec{r})\ \Phi_{\rm ext}\,(\vec{r})\ {\rm d}^3 r\,, \tag{5.107}$$

$$\Phi_{\rm ext}\,(\vec{r}) = \frac{1}{4\pi\epsilon_0} \int {\rm d}^3 r'\ \frac{1}{|\vec{r}-\vec{r}'|}\ \rho_{\rm ext}\,(\vec{r}')\ . \tag{5.108}$$

where $\rho_{\rm ext}\,(\vec{r}')$ is the "external" charge distribution, which is located at a large distance from the origin, while the "probe" charge distribution $\rho\,(\vec{r})$ is located near $\vec{r} \approx \vec{0}$. Hence, in particular,

$$\vec{\nabla}^2 \Phi_{\rm ext}\,(\vec{r})\Big|_{\vec{r}=0} = \sum_{i=1}^{3} \sum_{j=1}^{3} \delta_{ij}\ \frac{\partial^2 \Phi_{\rm ext}\,(\vec{r})}{\partial r_i \partial r_j}\bigg|_{\vec{r}=0} = 0\,, \tag{5.109}$$

because the potential $\Phi_{\rm ext}\,(\vec{r})$ is supposed to be due to charges external to the volume in which $\rho(\vec{r})$ is nonzero.

Because the sources of the potential are external to the volume containing the probe charge, the electric potential can be expanded in a Taylor series,

$$\Phi_{\rm ext}\,(\vec{r}) = \Phi_{\rm ext}\left(\vec{0}\right) + \sum_{i=1}^{3} r_i\ \frac{\partial \Phi_{\rm ext}\,(\vec{r}')}{\partial r_i'}\bigg|_{\vec{r}'=\vec{0}} + \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} r_i\, r_j\ \frac{\partial^2 \Phi_{\rm ext}\,(\vec{r}')}{\partial r_i' \partial r_j'}\bigg|_{\vec{r}'=\vec{0}} + \ldots\,. \tag{5.110}$$

Expressing the gradient of the external potential in terms of the electric field,

$$\vec{E}(\vec{0}) = -\ \frac{\partial \Phi\,(\vec{r}')}{\partial r_i'}\bigg|_{\vec{r}'=\vec{0}}\,, \tag{5.111}$$

we obtain the expansion of the potential energy in Cartesian coordinates,

$$\begin{aligned} W &= \Phi(\vec{0})\ \int \rho\,(\vec{r})\,{\rm d}^3 r - \vec{E}(\vec{0}) \cdot \int {\rm d}^3 r\ \vec{r}\,\rho\,(\vec{r}) \\ &\quad + \frac{1}{2}\ \sum_{i=1}^{3} \sum_{j=1}^{3}\ \frac{\partial^2 \Phi\,(\vec{r}')}{\partial r_i' \partial r_j'}\bigg|_{\vec{r}'=\vec{0}} \int {\rm d}^3 r\, r_i\, r_j\, \rho\,(\vec{r}) + \ldots \\ &= \Phi(\vec{0})\ Q - \vec{E}(\vec{0}) \cdot \vec{p} + \frac{1}{6}\ \sum_{i=1}^{3} \sum_{j=1}^{3}\ \frac{\partial^2 \Phi\,(\vec{r})}{\partial r_i \partial r_j}\bigg|_{\vec{r}=\vec{0}}\ Q_{ij} + \ldots\,. \end{aligned} \tag{5.112}$$

The first term is a kind of average potential energy, the second is the interaction of the electric dipole distribution with the applied electric field, and the third term gives the interaction of the quadrupole moment of the charge distribution with the gradient of the electric field. The formula for the total charge Q, the dipole moment vector $\vec{p}$, and the components of the quadrupole tensor Q_{ij}, have been given in Eq. (5.91). Equation (5.109) has been used in order to eliminate the term with $i = j$ in Eq. (5.91c).

5.1.9 Addition Theorem for Spherical Harmonics

Suppose that in the expansion of

$$\frac{1}{|\vec{r}-\vec{r}'|} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell+1}\ \frac{r_<^\ell}{r_>^{\ell+1}}\ Y_{\ell m}\,(\theta,\varphi)\ Y_{\ell m}^*\,(\theta',\varphi')\ , \tag{5.113}$$

we let $\vec{r}' = r'\hat{\mathrm{e}}_z$. Then, effectively, we have $\theta' = 0$. Only the $m = 0$ terms will appear in the sum because

$$Y_{\ell m}\,(0, \varphi') = 0\,, \qquad m \neq 0\,. \tag{5.114}$$

This holds because the associated Legendre polynomials $P_\ell^m(\cos\theta = 1)$ vanish save for the case $m = 0$, where $P_\ell^0(\cos\theta) = P_\ell(\cos\theta)$. In this case, we use the expression for $Y_{\ell m}\,(\theta, \varphi)$. In view of the equality $P_\ell(1) = P_\ell^0(1) = 1$, we have

$$\frac{1}{|\vec{r} - r'\,\hat{\mathrm{e}}_z|} = \sum_{\ell=0}^{\infty} \frac{4\pi}{2\ell+1}\,\frac{r_<^\ell}{r_>^{\ell+1}}\,Y_{\ell 0}\,(\theta, \varphi)\;\, Y_{\ell 0}^*\,(0, \varphi') \tag{5.115}$$

$$= \sum_{\ell=0}^{\infty} \frac{4\pi}{2\ell+1}\,\frac{r_<^\ell}{r_>^{\ell+1}}\,\sqrt{\frac{2\ell+1}{4\pi}}\,P_\ell(\cos\theta)\,\sqrt{\frac{2\ell+1}{4\pi}}\,P_\ell(1)\,. \tag{5.116}$$

So,

$$\frac{1}{|\vec{r} - \vec{r}'\,\hat{\mathrm{e}}_z|} = \sum_{\ell=0}^{\infty} \frac{r_<^\ell}{r_>^{\ell+1}}\,P_\ell\,(\cos\theta)\;. \tag{5.117}$$

In view of the equality

$$\frac{1}{|\vec{r} - \vec{r}'|} = \frac{1}{[r^2 + r'^2 - 2\,r\,r'\,\cos\theta]^{1/2}} = \sum_{\ell=0}^{\infty} \frac{r_<^\ell}{r_>^{\ell+1}}\,P_\ell\,(\cos\theta)\;, \tag{5.118}$$

we can now proceed in two steps. First, we observe that we have chosen $\vec{r}'$ to lie along the z axis somewhat arbitrarily. We can thus conclude that, more generally,

$$\frac{1}{|\vec{r} - \vec{r}'|} = \frac{1}{[r^2 + r'^2 - 2\,r\,r'\,\cos\gamma]^{1/2}} = \sum_{\ell=0}^{\infty} \frac{r_<^\ell}{r_>^{\ell+1}}\,P_\ell\,(\cos\gamma)\;, \qquad \gamma = \angle(\vec{r}, \vec{r}')\,, \qquad \cos\gamma = \hat{r}\cdot\hat{r}'\,. \tag{5.119}$$

The angle γ is between the vector locating the charge, $\vec{r}'$, and the vector locating the observation point, $\vec{r}$. On the other hand, the original multipole decomposition must still hold for the expression $1/|\vec{r} - \vec{r}'|$,

$$\frac{1}{|\vec{r} - \vec{r}'|} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell+1}\,\frac{r_<^\ell}{r_>^{\ell+1}}\,Y_{\ell m}\,(\theta, \varphi)\;\, Y_{\ell m}^*\,(\theta', \varphi')\;. \tag{5.120}$$

The equality of (5.119) and (5.120) has to hold for each ℓ component separately, and we obtain the addition theorem for spherical harmonics, which reads

Addition Theorem: $$P_\ell\,(\cos\gamma) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}\,(\theta, \varphi)\;\, Y_{\ell m}^*\,(\theta', \varphi')\;. \tag{5.121}$$

In particular,

$$P_1\,(\cos\gamma) = \hat{r}\cdot\hat{r}' = \frac{4\pi}{3} \sum_{m=-1}^{1} Y_{1m}\,(\theta, \varphi)\;\, Y_{1m}^*\,(\theta', \varphi')\;. \tag{5.122}$$

By expressing all direction cosines in spherical coordinates, we also obtain

$$\begin{aligned} \hat{r}\cdot\hat{r}' \equiv \cos\gamma &= \sin\theta\;\sin\theta'\;\{\cos\varphi\;\cos\varphi' + \sin\varphi\;\sin\varphi'\} + \cos\theta\cos\theta' \\ &= \sin\theta\sin\theta'\,\cos\,(\varphi - \varphi') + \cos\theta\cos\theta'\,. \end{aligned} \tag{5.123}$$

5.2 Green Function, Multipoles and Nontrivial Boundary Conditions

5.2.1 Laplace Equation for a Spherical Shell

We have previously encountered the functional decomposition of solutions of the Laplace equation as a convenient means of solving boundary problems with a specific symmetry. On the other hand, we have also discussed the general formalism of Dirichlet Green functions in order to describe both solutions of boundary value problems and to take into account the charge/source distributions within the probe volume V.

The primary aim of the current discussion is to solve boundary-value problems for a configuration with two spherical shells at radii $r = a$ and $r = b$, and to formulate the Green function for this configuration, using a multipole decomposition. A side effect of the current discussion is to show that it is actually possible to split a Dirichlet boundary-value problem with a nontrivial charge distribution, and nontrivial boundary conditions, into two problems, and to treat each of them separately. Indeed, for a specific geometry, that of concentric spheres, we will construct the Dirichlet Green function. We observe that Green's theorem in that case gives rise to two terms: the first describes the interaction of the sources and fields and the second describes the interaction of the boundary terms and the fields. For the first term, the calculation of the Dirichlet Green function is indispensable. For the second term, we have the choice of either treating it by the functional decomposition formalism, or by the Dirichlet Green function formalism. We call this approach a "hybrid" approach. In the formula

$$\Phi_D\left(\vec{r}'\right) = -\frac{1}{\epsilon_0}\int_V g_D\left(\vec{r},\vec{r}'\right)\ \rho\left(\vec{r}\right)\mathrm{d}^3r + \int_{\partial V}\Phi\left(\vec{r}\right)\vec{\nabla}g_D\left(\vec{r},\vec{r}'\right)\cdot\mathrm{d}\vec{S}\,, \tag{5.124}$$

we treat the term that involves an integration over ∂V using a series expansion, whereas the term with $\rho\left(\vec{r}\right)$ is treated using the Dirichlet Green function.

This leads to a combination of both approaches discussed previously, under the use of the superposition principle which allows us to choose the respective easiest method for each of the effects.

In order to treat the boundary-value problem (with trivial charge configuration $\rho(\vec{r}) = 0$), we start with the functional decomposition of the solution of the Laplace equation with azimuthal symmetry. We have previously discussed problems where we calculated a general solution to the Laplace equation

$$\vec{\nabla}^2\Phi(\vec{r}) = 0 \tag{5.125}$$

by expanding a suitable functional form into a complete set of functions, whose symmetry is adapted to the problem at hand. Let us now consider a problem where the boundary conditions and the charge densities have axial symmetry, i.e., they are independent of the azimuth angle φ. In that case, we can use the fact that the Legendre functions $P_\nu\left(\cos\theta\right)$ fulfill an orthogonality relation with respect to the integration measure

$$\langle f, g\rangle = \int_0^\pi \mathrm{d}\theta\ \sin\theta\ f^*(\theta)\, g(\theta)\,. \tag{5.126}$$

The potential can thus be conveniently expanded into the general form

$$\Phi\left(r,\theta\right) = \sum_{\ell=0}^{\infty} f_\ell\left(r\right)\ P_\ell\left(\cos\theta\right)\ . \tag{5.127}$$

Entire Range of the Polar Angle. Let us first treat a general problem with azimuthal symmetry (the potential is independent of the azimuthal angle φ) and with the polar angle covering $0 \leq \theta \leq \pi$, i.e., we

consider the general solution to the Legendre equation $\vec{\nabla}^2\Phi(\vec{r}) = 0$ for $\Phi(\vec{r}) = \Phi(r,\theta)$, where

$$\Phi(a,\theta) = f_a(\theta)\,, \qquad \Phi(b,\theta) = f_b(\theta) \tag{5.128}$$

are given as the boundary conditions. In this case, a convenient ansatz for the potential is then given by

$$\Phi\,(r,\theta) = \sum_{\ell=0}^{\infty} \left[\alpha_\ell\; r^\ell + \beta_\ell\; r^{-\ell-1}\right]\; P_\ell\,(\cos\theta)\;, \tag{5.129}$$

where we recall that the subscript of the Legendre polynomials (n) must be equal to the n that occurs in the exponents, for the Legendre equation to be fulfilled. In order to evaluate the coefficients, we need the orthogonality condition for the Legendre polynomials, which reads

$$\int_0^\pi P_\ell\,(\cos\theta)\;\; P_{\ell'}\,(\cos\theta)\;\; \sin\theta\,\mathrm{d}\theta = \int_{-1}^{1} P_\ell\,(u)\;\; P_{\ell'}\,(u)\;\; \mathrm{d}u = \frac{2\delta_{\ell\ell'}}{2\ell+1}\,. \tag{5.130}$$

Specifying the potential at $r = a$ and at $r = b > a$, we find that the coefficients satisfy the equations

$$\begin{aligned}
\Phi\,(a,\theta) &= \sum_{\ell=0}^{\infty} \left[\alpha_\ell\; a^\ell + \beta_\ell\; a^{-\ell-1}\right]\; P_\ell\,(\cos\theta) =: \sum_{\ell=0}^{\infty} I_\ell\,(a)\;\; P_\ell\,(\cos\theta)\;, \\
\Phi\,(b,\theta) &= \sum_{\ell=0}^{\infty} \left[\alpha_\ell\; b^\ell + \beta_\ell\; b^{-\ell-1}\right]\; P_\ell\,(\cos\theta) =: \sum_{\ell=0}^{\infty} I_\ell\,(b)\;\; P_\ell\,(\cos\theta)\;,
\end{aligned} \tag{5.131}$$

where we define

$$I_\ell(r) := \alpha_\ell\, r^\ell + \beta_\ell\, r^{-\ell-1}\,. \tag{5.132}$$

We now mulitply each side of Eq. (5.131) by $P_{\ell'}\,(\cos\theta)$, integrate over θ and then change the notation back according to the replacement $\ell' \to \ell$. Thus, we obtain

$$\frac{2\ell+1}{2} \int_0^\pi f_a(\theta)\; P_\ell\,(\cos\theta)\;\; \sin\theta\,\mathrm{d}\theta = I_\ell\,(a)\;, \tag{5.133a}$$

$$\frac{2\ell+1}{2} \int_0^\pi f_b(\theta)\; P_\ell\,(\cos\theta)\;\; \sin\theta\,\mathrm{d}\theta = I_\ell\,(b)\;. \tag{5.133b}$$

Now, on the one hand, we have defined the $I_\ell(a)$ and $I_\ell(b)$ according to Eq. (5.132). On the other hand, we can calculate $I_\ell(a)$ and $I_\ell(b)$ according to Eq. (5.133), because we assume that we have specified $f_a(\theta) = \Phi(a,\theta)$ and $f_b(\theta) = \Phi(b,\theta)$ for the two boundaries. Then, the $I_\ell(a)$ and $I_\ell(b)$ are known, and

$$\alpha_\ell \;=\; \frac{a^{\ell+1}\; I_\ell\,(a) - b^{\ell+1}\; I_\ell\,(b)}{a^{2\ell+1} - b^{2\ell+1}}\,, \tag{5.134a}$$

$$\beta_\ell \;=\; -\,(a\,b)^{\ell+1}\; \frac{b^\ell\, I_\ell\,(a) - a^\ell\, I_\ell\,(b)}{a^{2\ell+1} - b^{2\ell+1}}\,. \tag{5.134b}$$

In the limit $a \to 0$, we have $\alpha_\ell \to b^{-\ell} I_\ell\,(b)$ and $\beta_\ell \to 0$, while if $b \to \infty$ we have $\alpha_\ell \to 0$ and $\beta_\ell \to a^{\ell+1} I_\ell\,(a)$. In the latter cases, the number of applicable equations is halved, but the number of variables to be solved for is also halved. Equation (5.134) immediately leads to a solution of the Dirichlet problem given by the two concentric spheres, when the coefficients α_ℓ and β_ℓ are used in the ansatz (5.129).

Restricted Range of the Polar Angle. We now treat a problem with azimuthal symmetry and a restricted range for the polar angle, i.e., $0 \le \theta \le \beta < \pi$. Specifically, we consider a boundary-value problem of azimuthal symmetry, given by a convex hull of radius b, with the inner radius a. (Later, we shall let $a \to 0$.) The polar angle is restricted to the range $0 < \theta < \beta$. Furthermore, we assume boundary conditions which

imply that the entire surface at $\theta = \beta$ and $r \leq b$ is conducting and grounded, i.e., that the electrostatic potential there is zero.

The appropriate ansatz for the potential has to be modified from Eq. (5.129),

$$\Phi\,(r,\theta) = \sum_{\ell=0}^{\infty} \left(\alpha_\ell\; r^\ell + \beta_\ell\; r^{-\ell-1}\right)\; P_\ell\,(\cos\theta)\;, \tag{5.135}$$

to read

$$\Phi\,(r,\theta) = \sum_{\substack{\nu\,\in\,\mathbb{R} \\ P_\nu\,(\cos\beta)\,=\,0}} \left(\alpha_\nu\; r^\nu + \beta_\nu\; r^{-\nu-1}\right)\; P_\nu\,(\cos\theta)\;, \tag{5.136}$$

This change involves the replacement of the Legendre function $P_\ell(\cos\theta)$ by a Legendre function $P_\nu(\cos\theta)$ of non-integer subscript. Furthermore, the exponentials of r^ℓ and $r^{-\ell-1}$ are changed to r^ν and $r^{-\nu-1}$, respectively. The simultaenous change ensures that the Laplace equation again is fulfilled by all functions of the basis set used. We recall that the Legendre polynomials $P_\ell(u)$ fulfill the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}u}\,(1-u^2)\,\frac{\mathrm{d}}{\mathrm{d}u}P_\ell(u) + \ell(\ell+1)\;P_\ell(u) = 0\,. \tag{5.137}$$

So far, we have defined $P_\ell(u)$ only for integer ℓ. However, if we could define a Legendre function $P_\nu(u)$ for general $\nu \in \mathbb{R}$, then we could formulate the general ansatz for the solution in terms of Eq. (5.136). Let us therefore assume that there are Legendre functions that fulfill the equation

$$\frac{\mathrm{d}}{\mathrm{d}u}\,(1-u^2)\,\frac{\mathrm{d}}{\mathrm{d}u}P_\nu(u) + \nu(\nu+1)\;P_\nu(u) = 0\,. \tag{5.138}$$

for general ν. Indeed, this is possible, but we need the concept of the so-called hypergeometric function in order to grasp the idea. The Gaussian hypergeometric function is given by the series

$${}_2F_1(a,b,c,z) = \sum_{n=0}^{\infty} \frac{(a)_n\,(b)_n}{(c)_n}\;\frac{z^n}{n!} = \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(a)}\;\frac{\Gamma(b+n)}{\Gamma(b)}\;\frac{\Gamma(c)}{\Gamma(c+n)}\;\frac{z^n}{n!}\,, \tag{5.139}$$

where $(a)_n = \Gamma(a+n)/\Gamma(a)$ is a so-called Pochhammer symbol. For integer n, the Pochhammer symbol $(z)_n$ is given by

$$(z)_n = z\;(z+1)\;(z+2)\cdots(z+n-1) = \frac{(z+n-1)!}{(z-1)!} = \frac{\Gamma(z+n)}{\Gamma(z)}\,. \tag{5.140}$$

The Γ function is defined as

$$\Gamma(x) = \int_0^\infty t^{x-1}\;\exp(-t)\,\mathrm{d}t\,, \qquad \Gamma(x+1) = x\,\Gamma(x)\,, \qquad \Gamma(n+1) = n!\,. \tag{5.141}$$

The hypergeometric series generalizes the geometric series

$$\sum_{n=0}^{\infty} z^n = \frac{1}{1-z} \quad \rightarrow \quad \sum_{n=0}^{\infty} (\text{nontrivial-prefactors})\;\times\; z^n = \sum_{n=0}^{\infty} \frac{(a)_n\,(b)_n}{(c)_n\,n!}\;z^n\,. \tag{5.142}$$

The functions in Eqs. (5.142), (5.143) and (5.148) are defined by their Taylor expansions within the circle convergence ($|z| < 1$ and $|x| < 1$), and by analytic continuation elsewhere in the complex plane. We leave it to the reader to find the location of the branch cuts in the complex plane. We also note that in the case $a = b = c = 1$, the hypergeometric series reduces to the geometric series,

$$(1)_n = \frac{\Gamma(1+n)}{\Gamma(1)} = \Gamma(n+1) = n!\,, \qquad {}_2F_1(1,1,1,z) = \sum_{n=0}^{\infty} \frac{(1)_n\,(1)_n}{(1)_n\,n!}\;z^n = \sum_{n=0}^{\infty} z^n = \frac{1}{1-z}\,. \tag{5.143}$$

When the first argument (parameter) of the hypergeometric function is a negative integer, then the series actually terminates. This can be seen as follows. Let us consider the term with $n = 2$ in a hypergeometric series with $a = -3$. Then,

$$(-3)_2 = \frac{\Gamma(-3+2)}{\Gamma(-3)} = \frac{\Gamma(-1)}{\Gamma(-3)} = \frac{(-2)\,\Gamma(-2)}{\Gamma(-3)} = \frac{(-2)\,(-3)\,\Gamma(-3)}{\Gamma(-3)} = 6\,. \tag{5.144}$$

Actually, since neither $\Gamma(-3)$ nor $\Gamma(-1)$ is finite, we should actually define the Pochhammer symbol by the limiting process

$$\lim_{\epsilon\to 0}(-3+\epsilon)_{2+\epsilon} = \lim_{\epsilon\to 0}\frac{(-2+\epsilon)\,(-3+\epsilon)\,\Gamma(-3+\epsilon)}{\Gamma(-3+\epsilon)} = 6\,. \tag{5.145}$$

However, when $n = 4$, then

$$(-3)_4 = \frac{\Gamma(-3+4)}{\Gamma(-3)} = \frac{\Gamma(1)}{\Gamma(-3)} = \frac{1}{\infty} = 0\,. \tag{5.146}$$

In general, if $a = -\ell$ with integer ℓ, then the hypergeometric series is a polynomial in z of order ℓ. Because the Legendre polynomial P_ℓ is of order ℓ, we expect that it is represented by a terminating hypergeometric function with $a = -\ell$. Furthermore, we know that the Legendre function of the second kind $Q_\ell(u)$ has the form

$$Q_\ell\,(u) = \frac{P_\ell(u)}{2}\ln\left(\frac{1+u}{1-u}\right) + \mathcal{Q}_\ell(u) = P_\ell(u)\,\mathrm{arctanh}\,(u) + \mathcal{Q}_\ell(u)\,, \tag{5.147a}$$

$$\mathcal{Q}_0\,(u) = 0\,, \qquad \mathcal{Q}_1\,(u) = -1\,, \qquad \mathcal{Q}_2\,(u) = -\frac{3}{2}\,u\,, \qquad \mathcal{Q}_3\,(u) = -\frac{5}{2}\,u^2 + \frac{2}{3}\,. \tag{5.147b}$$

Here, $\mathcal{Q}_\ell(u)$ is a polynomial of order $\ell - 1$. Because $\mathrm{arctanh}(u)$ cannot be represented as a terminating polynomial, we expect that the associated Legendre function of the second kind, $Q_\ell^m(u)$, cannot be given in terms of a terminating hypergeometric series.

Without further ado, we now give the formulas for the Legendre functions of the first and second kind, for general non-integer arguments,

$$P_\ell^m\,(u) = \frac{1}{\Gamma(1-m)}\left(\frac{1+u}{1-u}\right)^{m/2}\,{}_2F_1\left(-\ell,\ell+1,1-m,\frac{1-u}{2}\right)\,, \tag{5.148a}$$

$$Q_\ell^m\,(u) \simeq \frac{\sqrt{\pi}\,\Gamma(\ell+m+1)}{2^{\ell+1}\,\Gamma(\ell+3/2)}\,\frac{(1-u^2)^{m/2}}{u^{\ell+m+1}}\,{}_2F_1\left(\frac{\ell+m+1}{2},\frac{\ell+m+2}{2},\ell+\frac{3}{2},\frac{1}{u^2}\right)\,. \tag{5.148b}$$

If we require that the solution of the Laplace equation be zero at $\theta = \beta$ and that it be finite for $0 \le \theta \le \beta$, then the most general solution will be a Legendre function of the first kind, $P_\nu\,(u = \cos\theta)$, where ν is not an integer. Legendre functions of the second kind are excluded because they diverge at $u = \cos\theta = 1$.

A word of caution is in order with regard to Eq. (5.148b). When taken at face value, this formula renders expressions for the $Q_\ell^m\,(u)$ which are valid when $|u| > 1$. This is natural because the argument of the hypergeometric series is $1/u^2$; the series converges for $|u| > 1$ and has to be analytically continued otherwise. Indeed, the result will be given in terms of the function

$$\mathrm{arctanh}(u) = \frac{1}{2}\,\ln\left(\frac{1+u}{1-u}\right)\,. \tag{5.149}$$

It is easy to find the analytic continuation of this function to the case $|u| > 1$. Namely,

$$\begin{aligned}\mathrm{arctanh}(u) &= \frac{1}{2}\,\ln\left(\frac{1+u}{1-u}\right) = \frac{1}{2}\,\ln\left(\frac{1+u}{u-1}\right) + \frac{\mathrm{i}\,\pi}{2} = \frac{1}{2}\,\ln\left(\frac{u+1}{u-1}\right) + \frac{\mathrm{i}\,\pi}{2}\\ &= \frac{1}{2}\,\ln\left(\frac{1+1/u}{1-1/u}\right) + \frac{\mathrm{i}\,\pi}{2} = \mathrm{arctanh}(1/u) + \frac{\mathrm{i}\,\pi}{2}\,.\end{aligned} \tag{5.150}$$

The Legendre function of the second kind $Q_\ell^m(u)$ is real rather than complex for real argument and parameters. Formula (5.148b) leads to expressions in terms of $\operatorname{arctanh}(1/u) = \operatorname{arccoth}(u)$, which is *a priori* defined for $|u| > 1$. However, if we replace

$$\operatorname{arctanh}(1/u) \quad \rightarrow \quad g(u) = \begin{cases} \operatorname{arctanh}(1/u) & |u| > 1 \\ \operatorname{arctanh}(u) & |u| < 1 \end{cases} \quad = \quad \operatorname{Re}(\operatorname{arctanh}(1/u))\,, \tag{5.151}$$

then we have accomplished the analytic continuation. Now, let us finally return to the analysis of our ansatz (5.136). If we set $m = 0$ in the relation (5.148a) for the P_ℓ^m, then we obtain

$$P_\ell(u) = P_\ell^0(u) = {}_2F_1\left(-\ell, \ell+1, 1; \frac{1-u}{2}\right). \tag{5.152}$$

So, we observe that the $P_\ell(u = \cos\theta)$ are generally expressed in terms of the hypergeometric functions ${}_2F_1(a, b, c; w)$, where we set $a = -\ell$, $b = 1 + \ell$, $c = 1$ and the argument is

$$w = \frac{1-\cos\theta}{2} = \sin^2\left(\frac{\theta}{2}\right). \tag{5.153}$$

When ℓ is not an integer (the parameter a is not a negative integer), then the function ${}_2F_1(-\ell, 1+\ell; 1, w)$ does not terminate and is an infinite series. We then have

$$P_\nu(\cos\theta) = P_\nu^0(u) = {}_2F_1\left(-\nu, 1+\nu;\ 1,\ \sin^2\left(\frac{\theta}{2}\right)\right) = \sum_{n=0}^{\infty} \frac{(-\nu)_n\,(\nu+1)_n}{(n!)^2}\,\sin^{2n}(\theta/2)\,. \tag{5.154}$$

We have required the solution of the Laplace equation to be zero at $\theta = \beta$ and to be finite for $0 \le \theta \le \beta$. If we now let $a \to 0$ in Eq. (5.136), then only the positive powers of r can survive,

$$\Phi(r, \theta) = \sum_{\substack{\nu > 0 \\ P_\nu(\cos\beta) = 0}} \alpha_\nu\, r^\nu\, P_\nu(\cos\theta)\,. \tag{5.155}$$

We require that $P_\nu(\cos\beta) = 0$. The relevant, suitable parameters

$$\nu = \{\nu_1, \nu_2, \dots\}\,, \qquad P_{\nu_n}(\cos\beta) = 0\,, \qquad n = 1, 2, \dots,, \tag{5.156}$$

can be determined by numerical investigation.

Fields near the Point of a Cone. The results of the last section can be applied to the problem of determining the fields and surface charge density near the tip of a conical conductor. In the region of interest, the surface of the cone makes an angle β with the z axis. We consider the region where the polar angle fulfills $0 < \theta < \beta$, i.e., from the top of the spherical coordinate system. For $\beta < \pi/2$, the region of interest is "inside" the cone while for $\beta > \pi/2$ the region is "outside" the conical surface.

If we take the cone to be at zero potential, then the leading term in the potential will be

$$\Phi(r, \theta, \varphi) \approx \Phi_0\, r^{\nu_1}\, P_{\nu_1}(\cos\theta)\,, \tag{5.157}$$

where ν_1 is determined by the condition that $\cos\beta$ is the first zero of $P_{\nu_1}(\cos\theta)$. For $0 < \nu < 3$ and $0 < \theta < \pi$, see Fig. 5.5. We note that Φ_0 does not automatically have the physical dimension of a potential, as dimensional analysis immediately shows. Near the tip of the cone (see Figs. 5.6 and 5.7), the electric field will have the components (we here appeal to the form the gradient operator in spherical coordinates)

$$E_r(r, \theta) = -\frac{\partial}{\partial r}\,\Phi(r, \theta, \varphi) \approx -\Phi_0\,\nu_1\, r^{\nu_1 - 1}\, P_{\nu_1}(\cos\theta)\,, \tag{5.158}$$

$$E_\theta(r, \theta) = -\frac{\partial}{r\,\partial\theta}\Phi_0\, r^{\nu_1}\, P_{\nu_1}(\cos\theta) \approx \Phi_0\, r^{\nu_1 - 1} \sin\theta\, P'_{\nu_1}(\cos\theta)\,. \tag{5.159}$$

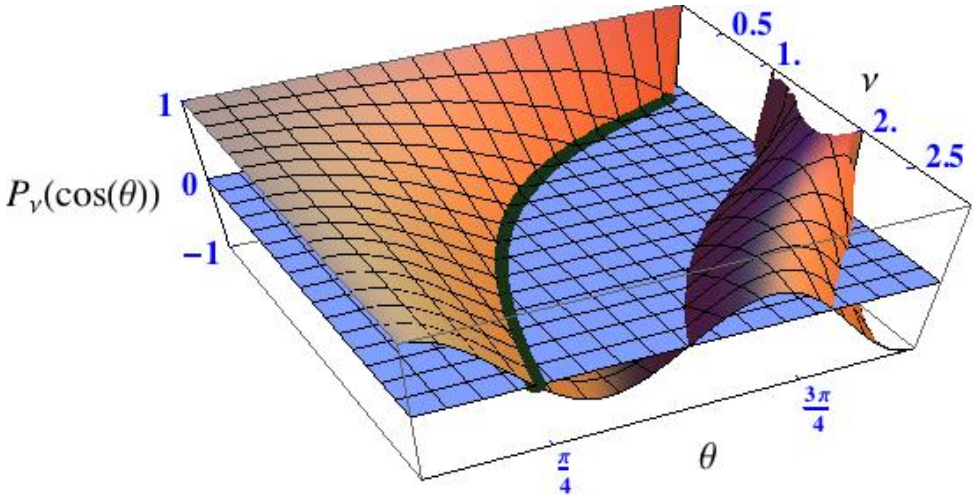

Figure 5.5: The plot shows $f(\nu,\theta) = P_\nu(\cos(\theta))$ for $0 < \nu < 3$ and $0 < \theta < \pi$, together with a plot of the trivial function $g(\nu,\theta) = 0$ in the same ν and θ interval. The zeros of the Legendre polynomials $P_\nu(\cos(\theta))$ are clearly visible, and we read off that $\nu_1 > 1$ for $\theta < \pi/2$, and that $\nu_1 < 1$ for $\theta > \pi/2$.

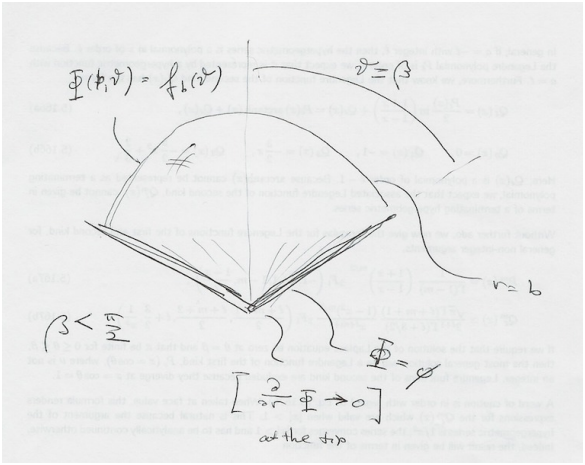

Figure 5.6: Boundary condition for a cone with $\beta < \pi/2$.

We are now interested in the surface charge density on the cone, i.e., on the surface defined by the equality $\theta = \beta$.

In that case, if we assume that the electric field vanishes outside of the geometric figure describe by the convex hull at $r = b$ and the conical surface described by $\theta = \beta$, then the surface charge density is given by (Gauss's theorem)

$$E_\theta = \hat{\mathrm{e}}_\theta \cdot \vec{E} = -\hat{n} \cdot \vec{E} = -\frac{\sigma(\vec{r})}{\epsilon_0}, \tag{5.160}$$

where $\hat{n}$ is normal to the conical surface defined by $\theta = \beta$. The minus sign is because the component of the electric field E_θ is defined to be in the direction of increasing θ, whereas the surface normal is defined to be

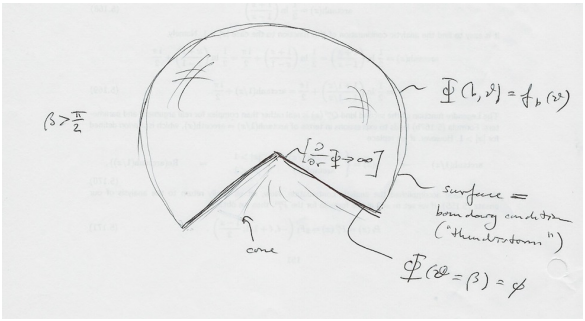

Figure 5.7: Boundary condition for a cone with $\beta > \pi/2$.

in the direction of decreasing θ. That is, $\hat{n} = -\hat{\mathrm{e}}_\theta$. Then,

$$\sigma\left(\vec{r}\right) \approx -\frac{1}{\epsilon_0}\, \Phi_0\, r^{\nu_1 - 1}\, \sin\beta\, P'_{\nu_1}\left(\cos\beta\right) . \tag{5.161}$$

We first consider the case with $\beta < \pi/2$. For this system, according to Fig. 5.5, $\nu_1 > 1$, and the fields and surface charges vanish as $r \to 0$, because the factor $r^{\nu_1 - 1}$ fulfills

$$r^{\nu_1 - 1} \to 0\,, \qquad \nu_1 > 1\,, \qquad \beta < \pi/2. \tag{5.162}$$

The geometry of this system would correspond to a conical hole in a conductor. As expected, the field does not readily penetrate a hole in a conductor. The alternate case has $\beta > \pi/2$. By numerical investigation, one may deduce that $\nu_1 < 1$ (see Fig. 5.5), i.e.

$$r^{\nu_1 - 1} \to \infty\,, \qquad \nu_1 < 1\,, \qquad \beta > \pi/2. \tag{5.163}$$

Clearly the fields and surface charge diverge as one approaches the tip of the cone. This amounts to a confirmation of the general wisdom that the fields are strong at pointed regions of a charged conductor.

5.2.2 Multipoles of the Green Function in a Spherical Shell

We have just considered the general solution of the Legendre equation under the boundary conditions given on concentric spherical shells with radii $r = a$ and $r = b > a$, using a functional decomposition. Let us try to do the same using the Dirichlet Green function. From the formula

$$\Phi_D\left(\vec{r}'\right) = -\frac{1}{\epsilon_0}\int_V g_D\left(\vec{r},\vec{r}'\right)\ \rho\left(\vec{r}\right)\mathrm{d}^3 r + \int_{\partial V} \Phi\left(\vec{r}\right)\vec{\nabla} g_D\left(\vec{r},\vec{r}'\right)\cdot \mathrm{d}\vec{S}\,, \tag{5.164}$$

we know that in order to solve a general problem with a nonvanishing charge distribution in between the spherical shells, we need the Dirichlet Green function which fulfills

$$\vec{\nabla}^2 g_D(\vec{r},\vec{r}') = \delta(\vec{r}-\vec{r}')\,, \qquad \text{and} \qquad g_D(\vec{r},\vec{r}') = 0 \quad \text{for} \quad \vec{r}\in\partial V\,. \tag{5.165}$$

In order to illustrate the Green function techniques, we consider systems which lie in a spherical shell $a \le r \le b$ bounded by conducting spherical shells. In this case, the potentials on the conductors are generally specified and the Dirichlet Green function is required.

In view of the symmetry, the following ansatz is required for the Green function,

$$g_D\left(\vec{r},\vec{r}'\right)=\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} g_\ell\left(r;r'\right)\; Y_{\ell m}\left(\theta,\varphi\right)\; Y^*_{\ell m}\left(\theta',\varphi'\right)\;, \tag{5.166}$$

which is the same as for the free Green function made in Eq. (5.71). We proceed as in the case of the ordinary Green function, i.e., we exclude the value at $r=r'$ and obtain two homogeneous equations, one for $a\le r<r'$ and the other for $r'<r\le b$. Unlike in the case of the free Green function, we can now combine the solutions regular at the origin and those regular at infinity, and combine them in such a way that they fulfill the homogeneous equation defining the Green function everywhere expect at $\vec{r}=\vec{r}'$. We then adjust the coefficients such as to ensure that $g_\ell\left(r;r'\right)=0$ at the surface of the conductor. It turns out that a suitable combination is

$$g_\ell\left(r,r'\right) = \alpha_\ell\left(r'\right)\;\left[\frac{r^\ell}{r'^{\,\ell+1}}-\frac{a^{2\ell+1}}{\left(r\,r'\right)^{\ell+1}}\right]\;,\qquad a\le r<r'\,, \tag{5.167a}$$

$$g_\ell\left(r,r'\right) = \beta_\ell\left(r'\right)\;\left[-\frac{\left(r\,r'\right)^\ell}{b^{2\ell+1}}+\frac{r'^\ell}{r^{\ell+1}}\right]\;,\qquad r'<r\le b\,. \tag{5.167b}$$

For $a\to 0$ and $b\to\infty$, both of these equations reproduce the structure encountered for the free Green function. Furthermore, the g_ℓ also fulfill

$$g_\ell\left(r,r'\right)=0\quad\text{at}\quad r=a,b\,. \tag{5.168}$$

Continuity of $g_\ell\left(r;r'\right)$ at $r=r'$ requires that

$$\alpha_\ell\left(r'\right)\;\left[\frac{1}{r'}-\frac{a^{2\ell+1}}{\left(r'\right)^{2\ell+2}}\right]-\beta_\ell\left(r'\right)\left[-\frac{\left(r'\right)^{2\ell}}{b^{2\ell+1}}+\frac{1}{r'}\right]=0\,. \tag{5.169}$$

In order to satisfy the differential equation

$$\vec{\nabla}^2 g_D(\vec{r},\vec{r}')=\delta^{(3)}(\vec{r}-\vec{r}')\,, \tag{5.170}$$

one needs to integrate Eq. (5.167) from $r=r'-\epsilon$ to $r=r'+\epsilon$. This procedure results in the following equation,

$$\alpha_\ell\left(r'\right)\;\left[\frac{\ell}{r'}+\frac{\left(\ell+1\right)\;a^{2\ell+1}}{r'^{\;2\ell+2}}\right]+\beta_\ell\left(r'\right)\;\left[\frac{\ell\;r'^{2\ell}}{b^{2\ell+1}}+\frac{\left(\ell+1\right)}{r'}\right]=-\frac{1}{r'}\,. \tag{5.171}$$

The two Eqs. (5.169) and (5.171) can be solved for $\alpha_\ell\left(r'\right)$ and $\beta\ell\left(r'\right)$,

$$\alpha_\ell\left(r'\right) = -\frac{1}{2\ell+1}\;\frac{1-\left(r'/b\right)^{2\ell+1}}{1-\left(a/b\right)^{2\ell+1}}\,, \tag{5.172a}$$

$$\beta_\ell\left(r'\right) = -\frac{1}{2\ell+1}\;\frac{1-\left(a/r'\right)^{\;2\ell+1}}{1-\left(a/b\right)^{2\ell+1}}\,, \tag{5.172b}$$

giving the result

$$g_D\left(\vec{r};\vec{r}'\right) = -\sum_{\ell=0}^{\infty}\frac{\left[b^{2\ell+1}-r_>^{2\ell+1}\right]\;\left[r_<^{2\ell+1}-a^{2\ell+1}\right]}{\left(2\ell+1\right)\left(b^{2\ell+1}-a^{2\ell+1}\right)\;\left(r\;r'\right)^{\ell+1}}\sum_{m=-\ell}^{\ell} Y_{\ell m}\left(\theta,\varphi\right)\;Y^*_{\ell m}\left(\theta',\varphi'\right)\;, \tag{5.173a}$$

$$\Phi_D\left(\vec{r};\vec{r}'\right) = \frac{q}{\epsilon_0}\sum_{\ell=0}^{\infty}\frac{\left[b^{2\ell+1}-r_>^{2\ell+1}\right]\;\left[r_<^{2\ell+1}-a^{2\ell+1}\right]}{\left(2\ell+1\right)\left(b^{2\ell+1}-a^{2\ell+1}\right)\;\left(r\;r'\right)^{\ell+1}}\sum_{m=-\ell}^{\ell} Y_{\ell m}\left(\theta,\varphi\right)\;Y^*_{\ell m}\left(\theta',\varphi'\right)\;. \tag{5.173b}$$

We recall once more that these quantities satisfy the equations

$$\vec{\nabla}^2\ \Phi_{\vec{r}'}\left(\vec{r}\right) = -\frac{1}{\epsilon_0}\ q\ \delta^{(3)}(\vec{r}-\vec{r}')\,, \qquad \vec{\nabla}^2\ g_D\left(\vec{r},\vec{r}'\right) = \delta^{(3)}(\vec{r}-\vec{r}')\,, \tag{5.174}$$

and they vanish on the two concentric spheres at $r = a$ and at $r = b$. Two remarks are in order here. We have considered a system with an inner shell of radius a and an outer shell of radius b, both held at a constant zero potential. If $a = 0$, this gives the Green function for the system confined to lie inside a spherical shell of radius b, while if $b \to \infty$, this is the Green's function for the system confined to lie outside a spherical shell of radius a.

5.2.3 Sources and Fields in a Spherical Shell

Let us consider grounded concentric spheres (held at zero potential), with radii $a < b$, separated by a uniformly charged annulus (ring) with total charge Q_0. The annulus is located in the plane $\theta = \pi/2$, i.e. it is stretched between the two concentric spherical shells. The problem is to determine the total charges on the spherical surfaces $r = a$ and $r = b$. We proceed in the following steps. First, we calculate the potential in the immediate vicinity of the concentric spheres, due to the uniformly charged annulus, with the use of the Dirchlet Green function just derived. (On the concentric spheres, the potential is of course zero, by virtue of the boundary conditions imposed on the concentric spheres, but this statement does not hold for the immediate vicinity of the spheres.) Then, we relate the surface charge density on the spheres to the normal component of the electric field on those surfaces and integrate. The result is the total charge on the two concentric surfaces.

The surface charge density on the ring between the spheres is

$$\sigma_0 = \frac{Q_0}{\pi\ \left(b^2 - a^2\right)}\,. \tag{5.175}$$

The charge density on the annulus therefore is (for the purposes of the θ' integration, we can assume that r' is a constant)

$$\rho\left(\vec{r}'\right) = \sigma_0\ \delta\left(z'\right) = \sigma_0\ \delta\left(r'\ \cos\theta'\right) = \frac{\sigma_0}{r'}\ \delta\left(\cos\theta'\right)\,, \qquad a \le r \le b, \tag{5.176}$$

and the boundary conditions are $\Phi\left(r = a, \theta, \varphi\right) = \Phi\left(r = b, \theta, \varphi\right) = 0$. With the given boundary conditions and the azimuthal symmetry, we have (the two overall minus signs of the Dirichlet Green function and of the formula that gives the potential, compensate each other)

$$\begin{aligned}
\Phi\left(r,\theta,\varphi\right) &= -\frac{1}{\epsilon_0}\int_{a\le r'\le b} g_D\left(\vec{r};\vec{r}'\right)\ \rho\left(\vec{r}'\right)\,\mathrm{d}^3r' \\
&= \frac{1}{\epsilon_0}\ \int_{a\le r'\le b}\ \sum_{\ell=0}^{\infty}\ \frac{\left[b^{2\ell+1} - r_>^{2\ell+1}\right]\ \left[r_<^{2\ell+1} - a^{2\ell+1}\right]}{\left(2\ell+1\right)\left(b^{2\ell+1} - a^{2\ell+1}\right)\ \left(r\ r'\right)^{\ell+1}}\ \sum_{m=-\ell}^{\ell} Y_{\ell m}\left(\theta,\varphi\right)\ Y_{\ell m}\left(\theta',\varphi'\right)^*\ \frac{\sigma_0}{r'}\ \delta\left(\cos\theta'\right)\ \mathrm{d}^3r'\,. \\
&= \frac{1}{\epsilon_0}\ \int_{a\le r'\le b}\ \sum_{\ell=0}^{\infty}\ \frac{\left[b^{2\ell+1} - r_>^{2\ell+1}\right]\ \left[r_<^{2\ell+1} - a^{2\ell+1}\right]}{\left(2\ell+1\right)\left(b^{2\ell+1} - a^{2\ell+1}\right)\ \left(r\ r'\right)^{\ell+1}}\ \left(\sqrt{\frac{2\ell+1}{4\pi}}\right)^2 \\
&\qquad \times P_\ell(\cos\theta)\ P_\ell(\cos\theta')\ \frac{\sigma_0}{r'}\ \delta\left(\cos\theta'\right)\ r'^2\mathrm{d}r'\ (2\pi)\ \mathrm{d}\cos\theta' \\
&= \frac{\sigma_0}{2\,\epsilon_0}\ \sum_{\ell=0}^{\infty}\ \frac{P_\ell\left(\cos\theta\right)\ P_\ell\left(0\right)}{b^{2\ell+1} - a^{2\ell+1}}\ \int_a^b \mathrm{d}r'\ r'\frac{\left(b^{2\ell+1} - r_>^{2\ell+1}\right)\ \left(r_<^{2\ell+1} - a^{2\ell+1}\right)}{\left(r\ r'\right)^{\ell+1}}\,.
\end{aligned} \tag{5.177}$$

The integral over r' can be carried out for the first few ℓ by an explicit calculation, where we use the general identity

$$\int_a^b \mathrm{d}r'\, f(r_<, r_>) = \int_a^r \mathrm{d}r'\, f(r', r) + \int_r^b \mathrm{d}r'\, f(r, r')\,. \tag{5.178}$$

The result for the first two novanishing terms is

$$\Phi(r,\theta,\varphi) = \frac{\sigma_0}{\epsilon_0}\,\frac{(a-r)\,(r-b)}{4\,r} - \frac{5\sigma_0}{32\epsilon_0}\,\frac{b^4\,(b-r)\,r^4 + a^5\,(b^4-r^4) + a^4(r^5-b^5)}{(b^5-a^5)\,r^3}\,(3\cos^2\theta - 1) + \ldots \tag{5.179}$$

and is the sum of the monopole and quadrupole terms. The general result consists of the even multipoles,

$$\begin{aligned}\Phi(r,\theta,\varphi) = \frac{\sigma_0}{\epsilon_0} \sum_{\ell=0,2,4,\ldots}^{\infty} & \frac{(2\ell+1)\,\sqrt{\pi}\,P_\ell(\cos\theta)}{2\,\Gamma(\frac{1}{2}-\frac{1}{2}\ell)\,\Gamma(1+\frac{1}{2}\ell)} \\ & \times \frac{(b\,r)^{\ell+1}\,(b^\ell\,r - b\,r^\ell) + a^{2\ell+1}\,(b^{\ell+2} - r^{\ell+2}) + a^{\ell+2}\,(r^{2\ell+1} - b^{2\ell+1})}{r^{\ell+1}\,(b^{2\ell+1} - a^{2\ell+1})\,(\ell^2+\ell-2)}\,.\end{aligned} \tag{5.180}$$

For odd ℓ, the Γ function $\Gamma(\frac{1}{2}-\frac{1}{2}\ell)$ becomes singular and the contribution vanishes, but it is safer to restrict the terms over which the sum is being carried out, explicitly to the even multipoles. A plot of the resulting potential, obtained by summing the first 40 some multipoles, is given in Fig. 5.8. The plot shows the sum of the first 40 multipoles in the expression (5.180) for the solution of the charged annulus inside the two concentric, grounded, spherical shells. It is given in the xz plane. The annulus lies in the plane $z = 0$ and is located where the potential is large. As we cannot realistically plot the potential as a function of the three coordinates x, y and z, we have chosen the x and z coordinates. The potential is rotationally symmetric about the z axis.

If we are only interested in an integrated quantity, namely, the net charge on the inner and outer spheres, the calculation simplifies considerably. The net charge is proportional to the monopole moment of the charge distribution, and the monopole moment is naturally isolated in the calculation. Also, since the potential is zero on the boundaries by assumption, we only need to consider the immediate vicinity of the boundaries. This simplifies the algebra in the radial integrals considerably.

The charge on the inner surface of the outer sphere can be calculated as follows ($r_> = r$, and $r_< = r'$). We invoke a Gaussian cylinder surrounding the surface, and take into account that the outer layer is grounded, i.e., held at zero potential. Hence, the electric field outside of the concentric sphere vanishes. Furthermore, this implies that the contribution to the surface integral (through the Gaussian cylinder) comes exclusively from the "inner" region where the surface normal is $-\hat{e}_r$ (which points toward the outside of the surface). So, there isn't a "factor $1/2$ coming in from the other cap of the Gaussian cylinder" as one might otherwise

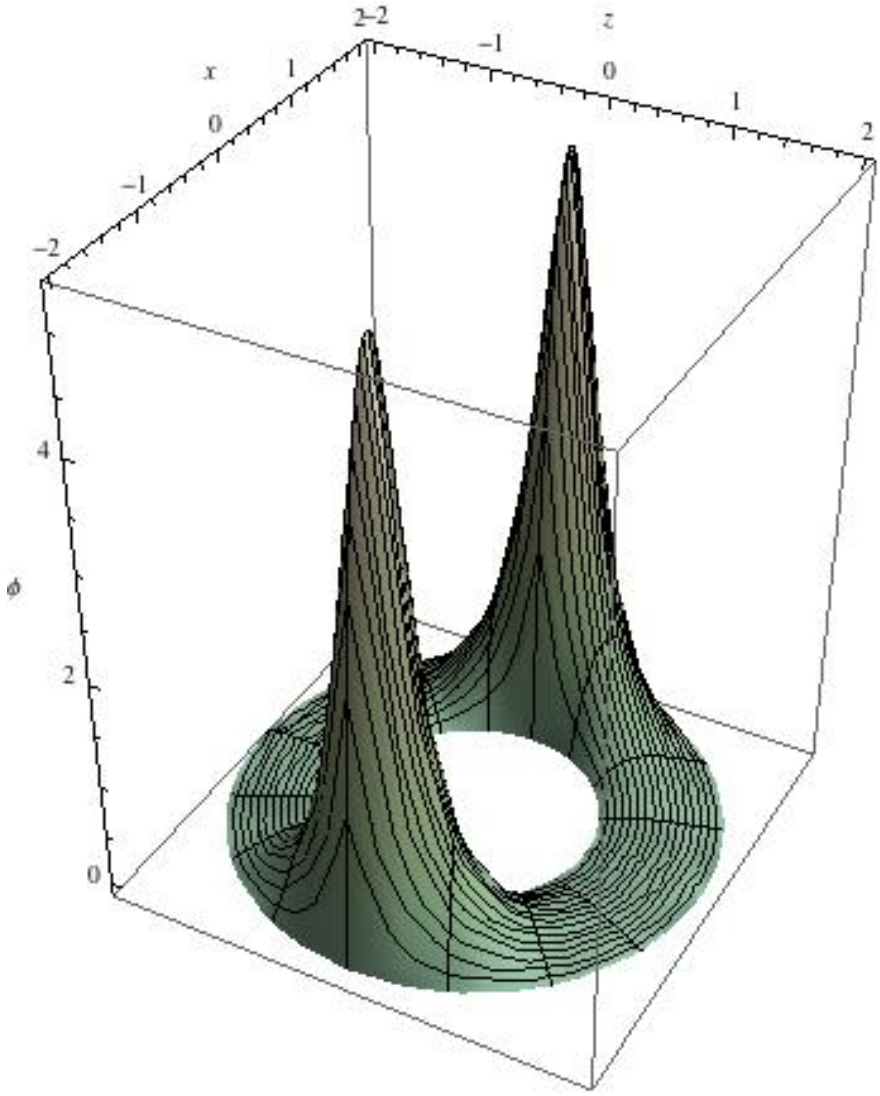

Figure 5.8: Plot of the potential (5.180) describing a uniformly charged annulus inside two grounded concentric spheres.

suggest. We have

$$
\begin{aligned}
Q_b &= \int_{r=b} \sigma(\vec{r})\, r^2\, \mathrm{d}\Omega = \int_{r=b} (-\epsilon_0\, E_r)\; r^2 \mathrm{d}\Omega = b^2\, \epsilon_0 \int \left.\frac{\partial \Phi\,(r,\theta,\varphi)}{\partial r}\right|_{r=b} \mathrm{d}\Omega \\
&\overset{r_>=r, r_<=r'}{=} \frac{\sigma_0\, b^2}{2}\,(2\pi) \sum_{\ell=0}^{\infty} \int_{-1}^{1} \left(\frac{P_\ell\,(\cos\theta)\, P_\ell\,(0)}{b^{2\ell+1} - a^{2\ell+1}} \mathrm{d}\cos\theta \right) \\
&\qquad \times \frac{\partial}{\partial r} \int_a^b r' \frac{\left(b^{2\ell+1} - r^{2\ell+1}\right)\left(r'^{2\ell+1} - a^{2\ell+1}\right)}{(r\, r')^{\ell+1}} \mathrm{d}r' \Bigg|_{r=b} \\
&\overset{\ell=0}{=} \frac{\sigma_0\, b^2}{2}\,(2\pi) \int_{-1}^{1} \left(\frac{P_0\,(\cos\theta)\, P_0\,(0)}{b-a}\, \mathrm{d}\cos\theta \right) \; \frac{\partial}{\partial r} \int_a^b \frac{b-r}{r}\, r' \frac{r'-a}{r'}\, \mathrm{d}r' \Bigg|_{r=b} \\
&= \frac{\sigma_0\, b^2}{2}\,(2\pi)\, \frac{2}{b-a} \left(\frac{\partial}{\partial r}\, \frac{b-r}{r}\Big|_{r=b} \right) \int_a^b (r'-a)\, \mathrm{d}r' \\
&= \frac{\sigma_0\, b^2}{2}\,(2\pi)\,(2)\, \frac{1}{b-a} \left(-\frac{b}{b^2} \right) \int_a^b (r'-a)\, \mathrm{d}r' \\
&= -\frac{2\pi\sigma_0\, b}{b-a}\, \frac{1}{2}\, (b-a)^2 = -\pi\sigma_0\, b\, (b-a)\,,
\end{aligned}
\tag{5.181}
$$

which has the right physical dimension. On the outer surface of the inner sphere, we have ($r_> = r'$, and $r_< = r$)

$$
\begin{aligned}
Q_a = \int_{r=a} \sigma(\vec{r})\, r^2\, \mathrm{d}\Omega &= \int_{r=a} (+\epsilon_0\, E_r)\; r^2 \mathrm{d}\Omega = -a^2\, \epsilon_0 \int \left.\frac{\partial \Phi\,(r,\theta,\varphi)}{\partial r}\right|_{r=a} \mathrm{d}\Omega \\
\overset{r_<=r, r_>=r'}{=} & -\frac{\sigma_0\, a^2}{2}\,(2\pi) \sum_{\ell=0}^{\infty} \int_{-1}^{1} \left(\frac{P_\ell\,(\cos\theta)\, P_\ell\,(0)}{b^{2\ell+1} - a^{2\ell+1}} \mathrm{d}\cos\theta \right) \\
& \times \frac{\partial}{\partial r} \int_a^b r' \frac{\left(b^{2\ell+1} - r'^{2\ell+1}\right)\left(r^{2\ell+1} - a^{2\ell+1}\right)}{(r\; r')^{\ell+1}} \mathrm{d}r' \Bigg|_{r=a} \\
\overset{\ell=0}{=} & -\frac{\sigma_0\, a^2}{2}\,(2\pi) \int_{-1}^{1} \left(\frac{P_0\,(\cos\theta)\, P_0\,(0)}{b-a}\; \mathrm{d}\cos\theta \right) \; \frac{\partial}{\partial r} \int_a^b r' \frac{b-r'}{r'}\; \frac{r-a}{r}\; \mathrm{d}r' \Bigg|_{r=a} \\
= & -\frac{\sigma_0\, a^2}{2}\,(2\pi)\, \frac{2}{b-a}\; \left(\frac{\partial}{\partial r}\; \frac{r-a}{r} \Bigg|_{r=a} \right) \int_a^b (b-r')\; \mathrm{d}r' \\
= & -\frac{\sigma_0\, a^2}{2}\,(2\pi)\,(2)\, \frac{1}{b-a}\; \left(\frac{a}{a^2}\right) \int_a^b (b-r')\; \mathrm{d}r' \\
= & -\frac{2\pi\sigma_0\, a}{b-a}\; \frac{1}{2}\; (b-a)^2 = -\pi\sigma_0\; a\; (b-a)\,.
\end{aligned}
\tag{5.182}
$$

The two charges Q_b and Q_a both have the same sign but are manifestly different, and the ratio is b/a. This is in line with intuition because of the following consideration: Namely, if the induced charge density on both concentric spheres were the same, then the ratio would be equal to the ratio of the surface areas, i.e., b^2/a^2. However, the average distance to the surface elements of the inner concentric sphere is smaller, and because the potential goes as the inverse distance, it is plausible that this change the ratio from b^2/a^2 to b/a. In the derivation, we have used the orthogonality of the Legendre polynomials in the form

$$
\int_{-1}^{1} P_\ell\,(u)\; P_\ell\,(0)\, \mathrm{d}u = \int_{-1}^{1} P_\ell\,(u)\, \mathrm{d}u = 2\; \delta_{\ell 0}\,. \tag{5.183}
$$