B POTENTIAL THEORY

B.1 *Potential theory*

Computing the field configuration $E_i(\boldsymbol{r})$ for a given distribution of electric charges $\rho(\boldsymbol{r})$ in the case of electrostatics requires the solution of the Poisson-equation through a convolution integral

$$\Delta\Phi(\boldsymbol{r}) = -4\pi\rho(\boldsymbol{r}) \quad \rightarrow \quad \Phi(\boldsymbol{r}) = \int_V \mathrm{d}V' \, \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} \tag{B.65}$$

with subsequently determining the gradient $E_i(\boldsymbol{r}) = -\partial_i\Phi(\boldsymbol{r})$. The reason for taking the detour over the potential Φ is that Poisson-problems of the form

$$\Delta\Phi(\boldsymbol{r}) = -4\pi\rho(\boldsymbol{r}) \tag{B.66}$$

are scalar and very well understood, with a plethora of solution methods. They map a single scalar source ρ onto a scalar field Φ, and from this perspective it is clear that the components of $E_i = -\partial_i\Phi$ can not be independent from each other, as they have to have a vanishing rotation, $\epsilon^{ijk}\partial_j E_k = 0$ in the static case. Please note that the inverse operation, i.e. determining the charge density ρ at a given position from the potential is straightforward: It suffices to compute the divergence of the gradient of the electric potential, $\Delta\Phi = \epsilon^{ij}\partial_i\partial_j\Phi$ to obtain ρ up to a factor of -4π.

Essentially, one needs to worry about three issues: (*i*) the inversion of the differential operator Δ for isolating Φ, which is achieved with the Green-function method, (*ii*) dealing with a possibly complicated geometry of the charge distribution ρ, and (*iii*) including boundary conditions typical for elliptical partial differential equations such as the Poisson-equation. The second issue is less severe and almost automatically taken care of if the first and third issue are solved: As the Poisson-equation is linear, the potential of an entire charge distribution should result from the superposition of the potentials generated by each infinitesimal element of charge.

B.2 *Systematic construction of Green-functions*

Formally, the solution to the Poisson-equation can be thought of as applying an inverse operator Δ^{-1} for isolating Φ from the relation $\Delta\Phi = -4\pi\rho$: The well-known convolution integral

$$\Phi = \int_V \mathrm{d}V' \, \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} \tag{B.67}$$

provides a solution to the Poisson-equation and therefore, consistency requires

$$\Phi = \Delta^{-1}\Delta\Phi = -4\pi\Delta^{-1}\rho. \tag{B.68}$$

In this sense, the convolution

$$\int_V \mathrm{d}V' \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \ldots \quad \text{is an inverse operation to} \quad \Delta[\ldots], \tag{B.69}$$

perfectly encapsulated in the relation

$$\Delta \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} = -4\pi\delta_{\mathrm{D}}(\boldsymbol{r}-\boldsymbol{r}'). \tag{B.70}$$

In this context, the integration kernel $1/|\boldsymbol{r}-\boldsymbol{r}'|$ is called the Green-function of the differential operator Δ (in three dimensions), and corresponds to the potential of a unit point charge. Although it is bad style (in my opinion), the notation Δ^{-1} can be used for denoting the convolution eqn. (B.69), and one formally solves the Poisson-equation by application of the Δ^{-1}-operator, $\Phi = \Delta^{-1}\Delta\Phi = -4\pi\,\Delta^{-1}\rho$, through convolution.

Up to this point, the approach was very intuitive: The Gauß-law suggests that the electrostatic field around a point charge should be $\propto 1/r^2$ and conservative, such that a potential exists. The potential has to have a scaling $\propto 1/r$ for its gradient to describe the electric field. But there should be a general way of constructing the Green-function Δ^{-1} for any differential operator Δ. For that purpose, one introduces the Fourier-transform of the potential

$$\Phi(\boldsymbol{k}) = \int_{\mathrm{V}} \mathrm{d}V\, \Phi(\boldsymbol{r}) \exp(-\mathrm{i}k_i r^i) \quad \leftrightarrow \quad \Phi(\boldsymbol{r}) = \int_{\mathrm{V}} \frac{\mathrm{d}^3k}{(2\pi)^3}\, \Phi(\boldsymbol{k}) \exp(+\mathrm{i}k_i r^i) \tag{B.71}$$

as well as of the charge density

$$\rho(\boldsymbol{k}) = \int_{\mathrm{V}} \mathrm{d}V\, \rho(\boldsymbol{r}) \exp(-\mathrm{i}k_i r^i) \quad \leftrightarrow \quad \rho(\boldsymbol{r}) = \int_{\mathrm{V}} \frac{\mathrm{d}^3k}{(2\pi)^3}\, \rho(\boldsymbol{k}) \exp(+\mathrm{i}k_i r^i) \tag{B.72}$$

Then, the Poisson-equation becomes

$$\begin{aligned} \Delta\Phi(\boldsymbol{r}) = \Delta \int_{\mathrm{V}} \frac{\mathrm{d}^3k}{(2\pi)^3}\, \Phi(\boldsymbol{k}) \exp(+\mathrm{i}k_i r^i) = \int_{\mathrm{V}} \frac{\mathrm{d}^3k}{(2\pi)^3}\, \Phi(\boldsymbol{k}) \Delta \exp(+\mathrm{i}k_i r^i) = \\ \int_{\mathrm{V}} \frac{\mathrm{d}^3k}{(2\pi)^3}\, \Phi(\boldsymbol{k})(-\gamma^{ab}k_a k_b) \exp(+\mathrm{i}k_i r^i) = -4\pi \int_{\mathrm{V}} \frac{\mathrm{d}^3k}{(2\pi)^3}\, \rho(\boldsymbol{k}) \exp(+\mathrm{i}k_i r^i) = -4\pi\rho(\boldsymbol{r}) \end{aligned} \tag{B.73}$$

as $\Delta = \gamma^{ab}\partial_a\partial_b$ acts on the plane wave $\exp(+\mathrm{i}k_i r^i)$ twice and generates a pre-factor $-\gamma^{ab}k_a k_b = -k^2$, for an isotropic medium for simplicity. Comparing the two Fourier-transforms suggests that

$$\Delta\Phi(\boldsymbol{r}) = -4\pi\rho(\boldsymbol{r}) \quad \rightarrow \quad k^2\Phi(\boldsymbol{k}) = 4\pi\rho(\boldsymbol{k}), \quad \text{solved by} \quad \Phi(\boldsymbol{k}) = \frac{4\pi}{k^2}\rho(\boldsymbol{k}) \tag{B.74}$$

Most interestingly, the (partial) differential equation has become a straightforward algebraic equation, which is readily solvable. Clearly, one can isolate Φ through division by $-k^2$ in Fourier-space, as illustrated by the diagram:

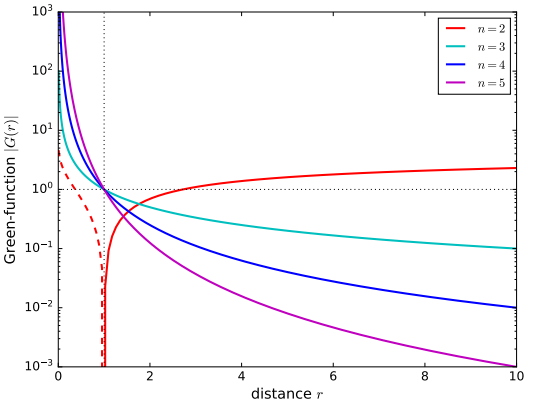


Figure 2: Green-functions $G(r)$ *of the Laplace-operator* Δ *in different dimensions* n.

$$\begin{array}{ccc} \Phi(\boldsymbol{r}) & \xleftarrow{\quad\mathcal{F}^{-1}\quad} & \Phi(\boldsymbol{k}) \\ \Big\downarrow{\scriptstyle \Delta} & & \Big\downarrow{\scriptstyle -\gamma^{ij}k_i k_j} \\ \rho(\boldsymbol{r}) & \xrightarrow{\quad\mathcal{F}\quad} & \rho(\boldsymbol{k}) \end{array} \tag{B.75}$$

which suggests that $\Phi = \mathcal{F}^{-1}\left(4\pi/k^2\ \mathcal{F}(\rho)\right)$, as the complication of solving the Poisson-equation is replaced by finding the Fourier-transform and its inverse. There are even performance advantages of taking the detour through Fourier-space, as there are very powerful and efficient Fourier-transform algorithms.

In fact, multiplications in Fourier-space are convolutions in real space, which implies for our case that the product between the Fourier-transformed Green-function $4\pi/k^2$ and the Fourier-transformed charge distribution $\rho(\boldsymbol{k}) = \mathcal{F}(\rho)$ yields the Fourier-transformed potential $\Phi(\boldsymbol{k})$ in this detour. At the same time, the Fourier-transform of $4\pi/k^2$ must be equal to $1/r$, which we already know to be the Green-function for Δ in 3 dimensions.

Let's repeat this construction for the Laplace-operator and derive an expression for the Green-function which is generalisable beyond $n = 3$ dimensions: In general, the Green-function $G(\boldsymbol{r}-\boldsymbol{r}')$ is defined as the potential for a unit point charge element, represented by a Dirac-δ_D, so the Poisson-equation needs to be fulfilled:

$$\Delta G(\boldsymbol{r}-\boldsymbol{r}') = -4\pi\delta_D(\boldsymbol{r}-\boldsymbol{r}') \tag{B.76}$$

Both the Green-function as well as the Dirac-δ_D have a Fourier representation:

$$G(\boldsymbol{r}-\boldsymbol{r}') = \int \frac{d^3k}{(2\pi)^3}\, G(\boldsymbol{k}) \exp(ik_i(\boldsymbol{r}-\boldsymbol{r}')^i) \quad \text{and} \quad \delta_D(\boldsymbol{r}-\boldsymbol{r}') = \int \frac{d^3k}{(2\pi)^3}\, \exp(ik_i(\boldsymbol{r}-\boldsymbol{r}')^i), \tag{B.77}$$

where δ_D has a constant amplitude in Fourier-space. Substituting into the Poisson-equation yields

$$\Delta G(\boldsymbol{r}-\boldsymbol{r}') = \Delta \int \frac{d^3k}{(2\pi)^3} G(\boldsymbol{k}) \exp(ik_i(\boldsymbol{r}-\boldsymbol{r}')^i) = \int \frac{d^3k}{(2\pi)^3} (-k^2) G(\boldsymbol{k}) \exp(ik_i(\boldsymbol{r}-\boldsymbol{r}')^i) =$$
$$-4\pi \int \frac{d^3k}{(2\pi)^3} \exp(ik_i(\boldsymbol{r}-\boldsymbol{r}')^i) = -4\pi\delta_D(\boldsymbol{r}-\boldsymbol{r}') \quad \text{(B.78)}$$

such that

$$G(\boldsymbol{k}) = \frac{4\pi}{k^2} \quad \text{(B.79)}$$

because each differentiation ∂_i generates a prefactor of ik_i. While the proportionality $\propto 1/k^2$ is valid in any number of dimensions, transforming back according to

$$G(\boldsymbol{r}-\boldsymbol{r}') = \int \frac{d^nk}{(2\pi)^n} G(\boldsymbol{k}) \exp(ik_i(\boldsymbol{r}-\boldsymbol{r}')^i) \quad \text{(B.80)}$$

leads to different results due to volume element $d^nk \propto k^{n-1}dk$ depending on dimensionality. In addition, 4π is just the full solid angle in three dimensions, and would need to be changed if the dimensionality is different.

B.3 *Green-theorems*

For showing the uniqueness of solutions to potential problems and for incorporating boundary conditions one needs the two Green-theorems, which are readily derived as particular cases of the Gauß-theorem. Defining

$$A_i(\boldsymbol{r}') = \phi(\boldsymbol{r}')\partial'_i\psi(\boldsymbol{r}') \quad \text{with two scalar fields } \phi,\ \psi \quad \text{(B.81)}$$

that all depend on the primed coordinate for convenience in the derivations later on, gives

$$\gamma^{ij}\partial'_i A_j = \gamma^{ij}\partial'_i\left(\phi\partial'_j\psi\right) = \gamma^{ij}\partial'_i\phi\,\partial'_j\psi + \phi\Delta'\psi \quad \text{(B.82)}$$

due to the Leibnitz-rule, and by writing $\gamma^{ij}\partial'_i\partial'_j = \Delta'$. Applying the Gauss-theorem yields the first Green-theorem

$$\int_V dV'\,\gamma^{ij}\partial'_i A_j = \int_V dV'\,\gamma^{ij}\partial'_i\left(\phi\partial'_j\psi\right) = \int_V dV'\,\left(\gamma^{ij}\partial'_i\phi\,\partial'_j\psi + \phi\Delta'\psi\right) =$$
$$\int_{\partial V} dS'_i\,\gamma^{ij}A_j = \int_{\partial V} dS'_i\,\gamma^{ij}\left(\phi\partial'_j\psi\right) \quad \text{(B.83)}$$

The right side of the first Green-theorem,

$$\int_V dV'\,\gamma^{ij}\partial'_i\left(\phi\partial'_j\psi\right) = \int_{\partial V} dS'_i\,\gamma^{ij}\left(\phi\partial'_j\psi\right), \quad \text{(B.84)}$$

can be interpreted as the scalar product of $\phi\partial'_j\psi$ with the surface normal dS'_i of the area element.

The second Green-theorem is obtained by interchanging the fields $\phi \leftrightarrow \psi$ in the first Green-theorem and by subtracting both expressions:

$$\int_V \mathrm{dV}' \left(\phi\gamma^{ij}\partial'_i\partial'_j\psi - \psi\gamma^{ij}\partial'_i\partial'_j\phi\right) = \int_{\partial V} \mathrm{dS}'_i\, \gamma^{ij}\left(\phi\partial'_j\psi - \psi\partial'_j\phi\right) \tag{B.85}$$

as the symmetric mixed term $\gamma^{ij}\partial'_i\psi\,\partial'_j\phi = \gamma^{ij}\partial'_i\phi\,\partial'_j\psi$ cancels.

The potential of an electrostatic problem is unique: For a given ρ there can be only a single potential Φ, defined up to an at most additive constant, which can be proved by contradiction. If there were two solutions

$$\Delta\Phi_1 = -4\pi\rho \quad \text{as well as} \quad \Delta\Phi_2 = -4\pi\rho \quad \rightarrow \quad \Delta\left(\Phi_1 - \Phi_2\right) = \Delta\delta = 0 \tag{B.86}$$

their difference $\delta = \Phi_1 - \Phi_2$ would fulfil the Laplace-equation $\Delta\delta = 0$, as shown by subtraction. Substituting δ into the first Green-theorem gives

$$\int_V \mathrm{dV}' \left[\delta\gamma^{ij}\partial'_i\partial'_j\delta - \gamma^{ij}\partial'_i\delta\partial'_j\delta\right] = \int_{\partial V} \mathrm{dS}'_i\, \gamma^{ij}\delta\partial'_j\delta = 0 \tag{B.87}$$

The surface-integral vanishes if proper boundary conditions are chosen on ∂V: Either, if $\Phi_1 = \Phi_2$ or $\delta = 0$ on ∂V is set (Dirichlet) or if $\partial'_j\Phi_1 = \partial'_j\Phi_2$ or $\partial'_j\delta = 0$ on ∂V (Neumann). With $\Delta'\delta = 0$ being zero because both Φ_1 and Φ_2 are solutions for the same source one arrives at

$$\int_V \mathrm{dV}'\, \gamma^{ij}\delta\partial'_j\delta = 0 \tag{B.88}$$

which implies that $\partial^{ij}\partial'_i\delta\partial'_j\delta = 0$, as the integrand is positive definite and must vanish over any specified volume. As a consequence, $\Phi_2 = \Phi_1 + \text{const}$ at most, and the constant must vanish for Dirichlet-conditions because of $\delta = 0$ on ∂V.

The solution to the Poisson-equation did not yet incorporate boundary conditions like specified values on surfaces or specified gradients. Setting

$$\psi(\boldsymbol{r}') \equiv \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \quad \rightarrow \quad \Delta'\psi(\boldsymbol{r}') = -4\pi\delta_D(\boldsymbol{r} - \boldsymbol{r}') \tag{B.89}$$

as well as

$$\phi(\boldsymbol{r}') \equiv \Phi(\boldsymbol{r}') \quad \rightarrow \quad \Delta'\phi(\boldsymbol{r}') = -4\pi\rho(\boldsymbol{r}') \tag{B.90}$$

suggests for the volume integrals

$$\int_V \mathrm{d}V' \left(\phi\gamma^{ij}\partial'_i\partial'_j\psi - \psi\gamma^{ij}\partial'_i\partial'_j\phi\right) =$$

$$\int_V \mathrm{d}V' \left(\Phi(\boldsymbol{r}')(-4\pi\delta_D(\boldsymbol{r}-\boldsymbol{r}')) + \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}4\pi\rho(\boldsymbol{r}')\right) =$$

$$-4\pi\Phi(\boldsymbol{r}) + 4\pi\int_V \mathrm{d}V' \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} \quad \text{(B.91)}$$

and for the surface integrals

$$\int_{\partial V} \mathrm{d}S'_i\gamma^{ij}\left(\phi\partial'_i\psi - \psi\partial'_j\phi\right) = \int_{\partial V} \mathrm{d}S'_i\gamma^{ij}\left(\Phi(\boldsymbol{r}')\partial'_j\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} - \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\partial'_j\Phi(\boldsymbol{r}')\right) \quad \text{(B.92)}$$

Assembling the entire expression gives the relation

$$\Phi(\boldsymbol{r}) = \int_V \mathrm{d}V' \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + \frac{1}{4\pi}\int_{\partial V} \mathrm{d}S'_i\,\gamma^{ij}\left(\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\partial'_j\Phi(\boldsymbol{r}') - \Phi(\boldsymbol{r}')\partial'_j\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\right) \quad \text{(B.93)}$$

with the volume integral reiterating the conventional way of computing Φ from ρ, augmented by two additional contributions, one representing ✈ Neumann-boundary conditions with $\nabla\Phi$ on ∂V and the second representing ✈ Dirichlet-boundary conditions with Φ on ∂V. If the boundary is at infinity, both $1/r\,\nabla\Phi$ and $\Phi\,\nabla 1/r$ tend to zero as $1/r^3$, so the first term is the only one to survive. Interestingly, the formula suggests that there can be a nontrivial potential Φ even though ρ might be zero: Then, the potential is determined by Φ and $\nabla\Phi$ on the boundary. It might be a surprisingly sensible question, if one can construct a charge distribution that replaces the boundary conditions in an otherwise unconstrained potential problem, and the question can be positively answered: Any potential Φ is linked to a distribution of sources ρ through the Poisson-equation $\Delta\Phi = -4\pi\rho$, so setting $\rho = -\Delta\Phi/(4\pi)$ would be consistent with a potential fulfilling the boundary conditions, which is exactly the method of ✈ mirror charges.

B.4 *Spherical multipole expansion*

The Green-function $1/|\boldsymbol{r}-\boldsymbol{r}'|$ is the correct convolution kernel for computing the potential Φ for any charge distribution ρ in fulfilment of the Poisson-equation $\Delta\Phi = -4\pi\rho$. But there might be cases where an approximate computation of Φ is sufficient, in particular because intuitively, any localised charge distribution should generate a Coulomb-like spherically symmetric $1/r$-potential at large distances, with deviations only appearing at smaller distances: This is shown in Fig. 3, where one of isopotential surfaces is given for a uniformly charged cube. With increasing distance (and correspondingly, lower values for Φ), the surfaces become more and more spherical, as expected from the Coulomb-potential of a point charge. The effect is more pronounced in Fig. 4, where the isocontours of the potential of a charge distribution with four equal charges in the corners of a tetrahedron is shown.

In fact, expanding the Green-function leads to

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} = \frac{1}{\sqrt{r^2 - 2rr'\mu + r'^2}} = \frac{1}{r}\frac{1}{\sqrt{1 - 2\frac{r'}{r}\mu + \frac{r'^2}{r^2}}} \tag{B.94}$$

where $\mu = \cos\theta$ is the cosine of the angle between $\boldsymbol{r}$ and $\boldsymbol{r}'$. If one assumes now that the observation point $\boldsymbol{r}$ is far away from the charge distribution (and $\boldsymbol{r}'$ points by definition of the convolution relation to every charge element), then $r \gg r'$ and the root can be expanded:

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} = \frac{1}{r}\sum_{\ell=0}^{\infty}\left(\frac{r'}{r}\right)^{\ell} \mathrm{P}_\ell(\mu) \tag{B.95}$$

where $\mathrm{P}_\ell(\mu)$ are the Legendre-polynomials. They follow explicitly from the relation

$$\frac{1}{\sqrt{1 - 2\mu x + x^2}} = \sum_{\ell=0}^{\infty} \mathrm{P}_\ell(\mu) x^\ell \tag{B.96}$$

by ℓ-fold differentiation with respect to $x = r'/r \ll 1$ and successive setting of $x = 0$. Explicitly, this would result in $\mathrm{P}_0(\mu) = 1$, $\mathrm{P}_1(\mu) = \mu$ and $\mathrm{P}_2(\mu) = (3\mu^2 - 1)/2$.

Now, one can bridge between the Legendre-polynomals $\mathrm{P}_\ell(\cos\gamma)$ and the spherical harmonics $\mathrm{Y}_{\ell m}(\theta, \varphi)$ with the addition theorem

$$\mathrm{P}_\ell(\cos\gamma) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{+\ell} \mathrm{Y}_{\ell m}(\theta,\varphi)\mathrm{Y}^*_{\ell m}(\theta',\varphi') \tag{B.97}$$

with γ being the angle between (θ, φ) and (θ', φ'). These spherical harmonics are waves on the surface of the sphere

$$\Delta \mathrm{Y}_{\ell m}(\theta,\varphi) = -\ell(\ell+1)\mathrm{Y}_{\ell m}(\theta,\varphi), \quad \text{analogous to} \quad \Delta \exp(\pm \mathrm{i} k_i r^i) = -\gamma^{ab}k_a k_b \exp(\pm \mathrm{i} k_i r^i) \tag{B.98}$$

so that ℓ plays the role of a wave number, and its inverse reflects the wave length (in radians) of the waves. The spherical harmonics (for details, see Sect. X.6) constitute therefore a harmonic system and are naturally related to Fourier-transforms, and generalise the idea of harmonic analysis to functions defined on the surface of a sphere.

Replacing the Legendre-polynomials by spherical harmonics leads to

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\frac{4\pi}{2\ell+1}\frac{r'^\ell}{r^{\ell+1}}\mathrm{Y}_{\ell m}(\theta,\varphi)\mathrm{Y}^*_{\ell m}(\theta',\varphi') \tag{B.99}$$

which can be substituted into the expression of the potential

$$\Phi(\boldsymbol{r}) = \int_{\mathrm{V}} \mathrm{d}V'\,\frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\frac{4\pi}{2\ell+1}\frac{1}{r^{\ell+1}}\mathrm{Y}_{\ell m}(\theta,\varphi) \times \int_{\mathrm{V}} \mathrm{d}V'\,\rho(\boldsymbol{r}')r'^\ell \mathrm{Y}^*_{\ell m}(\theta',\varphi'). \tag{B.100}$$

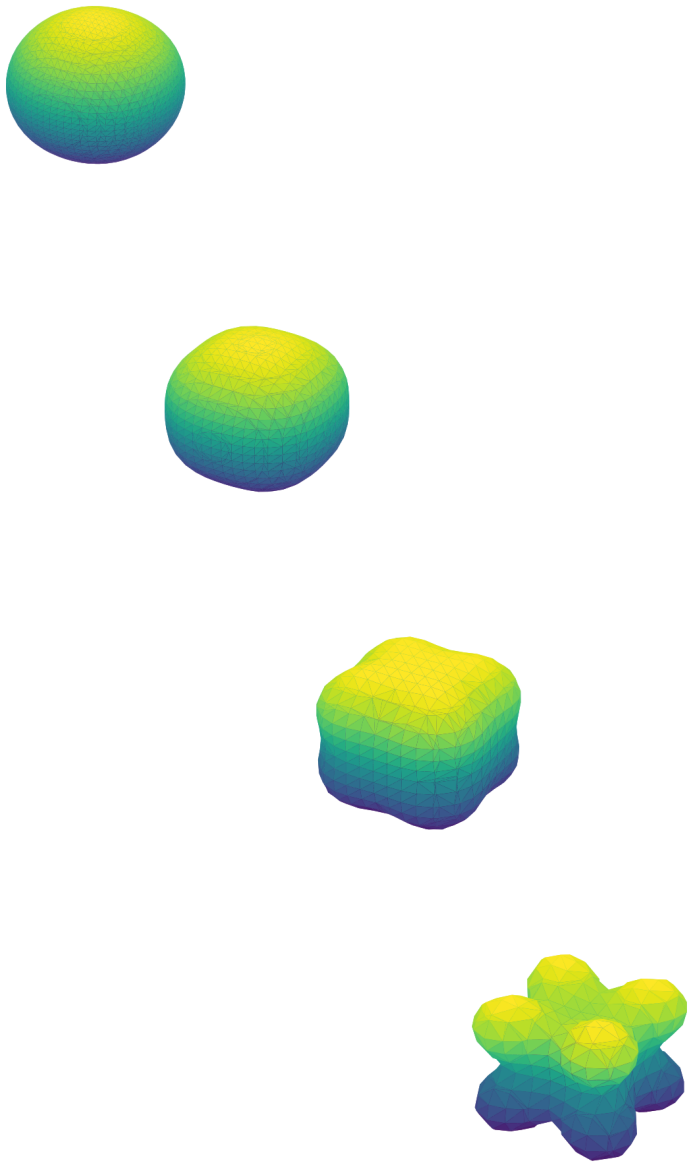


Figure 3: Isopotential surfaces of the potential sourced by eight equal charges, situated at the corners of a cube, at decreasing distance

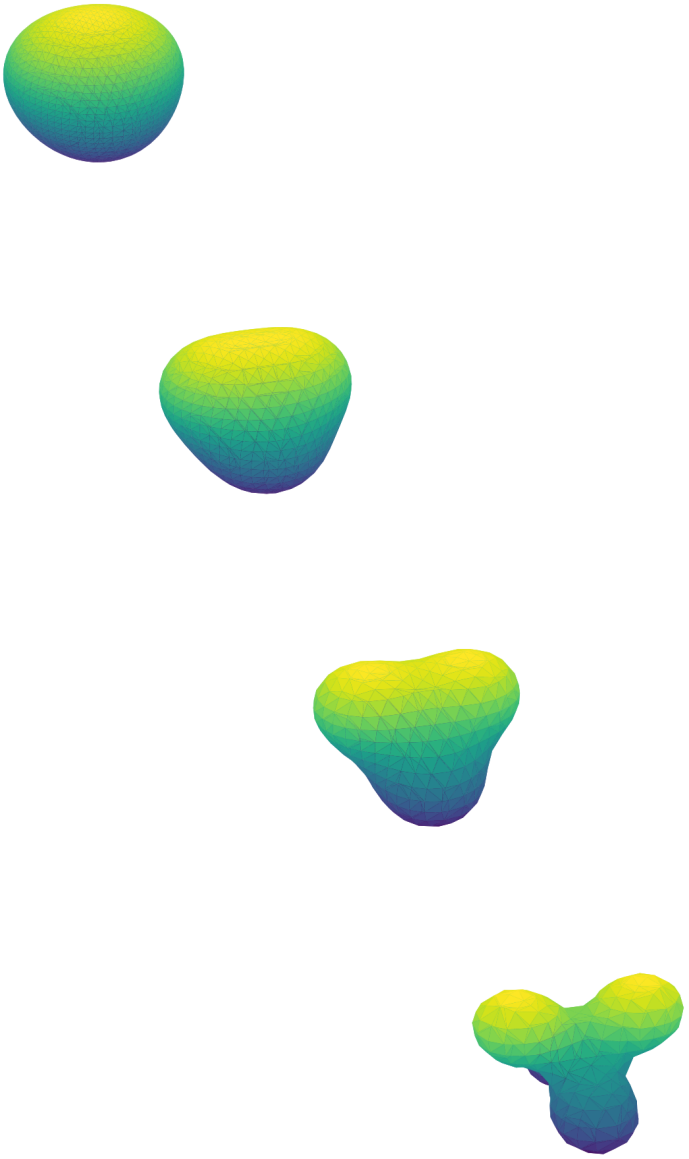


Figure 4: Isopotential surfaces of the potential sourced by four equal charges, situated at the corners of an tetrahedron, at decreasing distance

This formula is remarkable because it separates properties of the charge distribution from the field that it would generate: Sorting the variables into primed and unprimed leads to the definition of multipole moments $q_{\ell m}$

$$q_{\ell m} = \int_V \mathrm{d}V'\, \rho(\boldsymbol{r}') r'^{\ell} Y^*_{\ell m}(\theta', \varphi'). \tag{B.101}$$

The multipole moments are a complete characterisation of the charge distribution and contain information about the magnitude of the charge, the spatial size, the shape, asphericity and orientation. Each of the multipoles is an independent contribution to the potential Φ, whose influence decreases as $1/r^{\ell+1}$

$$\Phi(\boldsymbol{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \frac{4\pi}{2\ell+1} \frac{1}{r^{\ell+1}} Y_{\ell m}(\theta, \varphi) q_{\ell m}, \tag{B.102}$$

which is amazingly practical, as higher-order multipoles generate contributions to Φ which decay faster and faster with increasing distance. At large distances, only the lowest order multipole can contribute, and it is sensible to expect that this contribution should be a spherically symmetric potential determined by the total charge. In fact, there is only $m = 0$ permissible for $\ell = 0$, so that there is a single coefficient q_{00},

$$q_{00} = \int_V \mathrm{d}V' \underbrace{r'^0}_{=1} \rho(\boldsymbol{r}') \underbrace{Y^*_{00}(\theta', \varphi')}_{=\frac{1}{\sqrt{4\pi}}} = \frac{q}{\sqrt{4\pi}} \tag{B.103}$$

Therefore, the monopole q_{00} is the total charge of the system q, up to a factor of $1/\sqrt{4\pi}$. At large distances, this term would dominate the multipole expansion and generate a $1/r$-like contribution to the potential Φ, in agreement with intuition that the potential, viewed from a large distance of a somehow localised charge distribution, should have this form.

The dipole $\ell = 1$ allows the three choices $m = -1, 0, +1$, therefore, there are three dipole moments

$$q_{1m} = \int_V \mathrm{d}V'\, r' \rho(\boldsymbol{r}') Y^*_{1m}(\theta', \varphi') \tag{B.104}$$

whose fundamental functional form is that of "charge × distance", and carrying the sequence further one defines 5 quadrupole moments q_{2m} for $m = -2\ell, -\ell, 0, +\ell, +2\ell$

$$q_{2m} = \int_V \mathrm{d}V'\, r'^2 \rho(\boldsymbol{r}') Y^*_{2m}(\theta', \varphi') \tag{B.105}$$

with a fundamental scaling "charge × area", and it is obvious how this would generalise to higher order multipoles such as octupoles and hexadecupoles. The idea is always that the charge distribution is split up into coefficients $q_{\ell m}$ that by construction look for smaller and smaller structures and that are sensitive to the spatial extent (through the weighting with r'^{ℓ}) of the charge distribution, and to its asphericity and orientation (through projection onto the spherical harmonics $Y_{\ell m}(\theta', \varphi')$).

Formally, one needs the full set of multipole moments for writing down the multipole expansion, but there is a hermiticity constraint just as in the case of the Fourier-components of negative frequency for a real-valued function. Fundamentally, one has

$$Y^*_{\ell m}(\theta,\varphi) = (-1)^m Y_{\ell,-m}(\theta,\varphi) \tag{B.106}$$

which maps onto the relation

$$q^*_{\ell m} = \int_V \mathrm{d}V'\, r'^{\ell}\rho(\boldsymbol{r}')Y_{\ell m}(\theta',\varphi') = (-1)^m \int_V \mathrm{d}V'\, r'^{\ell}\rho(\boldsymbol{r}')Y^*_{\ell,-m}(\theta',\varphi') = (-1)^m q_{\ell,-m} \tag{B.107}$$

so that there are not $2\ell+1$ but rather only $\ell+1$ independent multipole coefficients for a real-valued charge distribution. With this realisation it is clear that the charged cube in Fig. 3 can only exhibit a monopole and an octupole at lowest order. While the monopole gives rise to a straightforward spherically symmetric Coulomb-potential, the octupole contribution falls of very quickly $\propto 1/r^4$, so that it only matters very close to the surface of the cube, and renders the isopotential surface non-spherical.

B.5 *Cartesian multipole expansion*

There is an alternative approach to multipole expansions in terms of Cartesian coordinates, where the Green-function of a charge distribution localised around the origin of the coordinate system is Taylor-expanded at $\boldsymbol{r}' = 0$ with respect to the variable $\boldsymbol{r}'$, while $\boldsymbol{r}$ is kept fixed:

$$G(\boldsymbol{r},\boldsymbol{r}') \simeq G\Big|_{\boldsymbol{r}'=0} + \partial'_i G\Big|_{\boldsymbol{r}'=0}(x')^i + \frac{1}{2!}\partial'_i\partial'_j G\Big|_{\boldsymbol{r}'=0}(x')^i(x')^j + \cdots \tag{B.108}$$

The necessary derivatives of $G(\boldsymbol{r},\boldsymbol{r}')$ at $\boldsymbol{r}' = 0$ are easily computed to be

$$G\Big|_{\boldsymbol{r}'=0} = \frac{1}{r}, \quad \partial'_i G\Big|_{\boldsymbol{r}'=0} = \frac{\gamma_{ia}x^a}{r^3}, \quad \text{and} \quad \partial'_i\partial'_j G\Big|_{\boldsymbol{r}'=0} = \frac{3\gamma_{ia}x^a\gamma_{jb}x^b - r^2\gamma_{ij}}{r^5} \tag{B.109}$$

using the explicit form of the Green-function in Cartesian coordinates

$$G(\boldsymbol{r},\boldsymbol{r}') = \left[\gamma_{ab}(\boldsymbol{r}-\boldsymbol{r}')^a(\boldsymbol{r}-\boldsymbol{r}')^b\right]^{-1/2}. \tag{B.110}$$

Here, we abbreviate $r^2 = \gamma_{ij}x^i x^j$ as the Euclidean norm of $\boldsymbol{r}$. Then, the potential Φ is given at $r \gg r'$ as

$$\Phi(\boldsymbol{r}) = \int_V \mathrm{d}V' \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} \simeq \int_V \mathrm{d}V'\rho(\boldsymbol{r}')\left[\frac{1}{r} + \frac{\gamma_{ia}x^a(x')^i}{r^3} + \frac{3\gamma_{ia}x^a\gamma_{jb}x^b - r^2\gamma_{ij}}{r^5}(x')^i(x')^j + \cdots\right] \tag{B.111}$$

Applying the integration to each term in the series while interchanging summation and integration gives

$$\Phi(\boldsymbol{r}) \simeq \frac{1}{r}\int_{\mathrm{V}} \mathrm{d}\mathrm{V}'\ \rho(\boldsymbol{r}') + \frac{x^a}{r^3}\int_{\mathrm{V}} \mathrm{d}\mathrm{V}'\ \rho(\boldsymbol{r}')\gamma_{ia}(x')^i + \\ \frac{1}{2!}\frac{3\gamma_{ia}x^a\gamma_{jb}x^b - r^2\gamma_{ij}}{r^5}\int_{\mathrm{V}} \mathrm{d}\mathrm{V}'\ \rho(\boldsymbol{r}')(x')^i(x')^j \quad \text{(B.112)}$$

where we can identify the Cartesian multipole moments: The total charge q in the first term, the dipole moment q_a in the second term, and the quadrupole moment in the last term. They contribute to the potential Φ with increasing powers of $1/r$, so that their influence at large distance decreases with multipole order.

There might be an aesthetic issue, as $3\gamma_{ai}x^a\gamma bjx^b - r^2\gamma ij$ is not mirrored in the primed coordinate in the quadrupole term, likewise one might be irritated why there seem to be six Cartesian multipole moments (There are 6 independent choices for i and j in the tensor $(x')^i(x')^j$) but only five in spherical coordinates (The index m can assume the 5 different values -2, -1, 0, 1 and 2 for $\ell = 2$). In order to remedy this issue, one adds a zero in the expression for the quadrupole moment

$$\frac{3\gamma_{ai}x^a\gamma_{jb}x^b - r^2\gamma_{ij}}{r^5}\int_{\mathrm{V}} \mathrm{d}\mathrm{V}'\left(\rho(\boldsymbol{r}')\,(x')^i(x')^j \underbrace{-r'^2\frac{\gamma^{ij}}{3} + \overbrace{r'^2\frac{\gamma^{ij}}{3}}^{\text{becomes zero}}}_{=0}\right) \quad \text{(B.113)}$$

The last term in particular can be simplified, as in its contraction with the prefactor one can write:

$$\frac{3\gamma_{ai}x^a\gamma_{jb}x^b - r^2\gamma_{ij}}{r^5}\int_{\mathrm{V}} \mathrm{d}\mathrm{V}'\ \rho(\boldsymbol{r}')r'^2\frac{\gamma^{ij}}{3} = 0 \quad \text{(B.114)}$$

because of $\gamma_{ai}\gamma_{bj}\gamma^{ij}x^ax^b = \gamma_{ab}x^ax^b = r^2$ and because $\gamma_{ij}\gamma^{ij} = \delta^i_i = 3$. Therefore, only the combination of the first two terms remain, explicitly

$$\frac{3\gamma_{ai}x^a\gamma_{bj}x^b - r^2\gamma_{ij}}{r^5}\int_{\mathrm{V}} \mathrm{d}\mathrm{V}'\ \rho(\boldsymbol{r}')\left(3(x')^i(x')^j - r'^2\gamma^{ij}\right) = \\ \frac{3x^ax^b - r^2\gamma^{ab}}{r^5}\int_{\mathrm{V}} \mathrm{d}\mathrm{V}'\ \rho(\boldsymbol{r}')\left(3\gamma_{ai}(x')^a\gamma_{bj}(x')^b - r'^2\gamma^{ab}\right) \quad \text{(B.115)}$$

establishing an identical structure in the quadrupole term. Summarising all terms then yields the final result for the potential

$$\Phi(\boldsymbol{r}) = \frac{q}{r} + q_i\frac{x^i}{r^3} + q_{ij}\frac{3x^ix^j - r^2\gamma^{ij}}{r^5} \quad \text{(B.116)}$$

with the monopole that shows the expected $1/r$-behaviour, followed by the dipole term with a fundamental scaling $\propto 1/r^2$ and an angular cosine-like behaviour en-

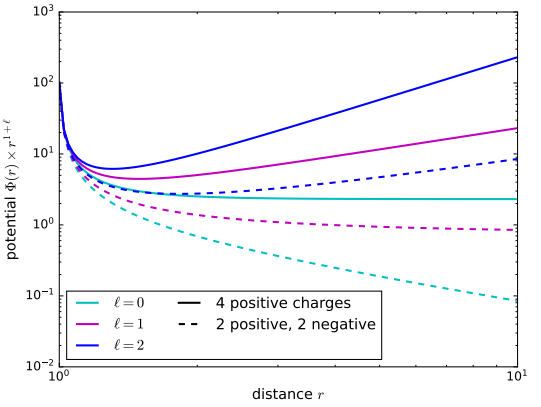


Figure 5: Potential Φ of the tetrahedron as a function of distance r, in the representation $\Phi \times r^{1+\ell}$, therefore, a flat section indicates a scaling $\Phi \propto 1/r^{1+\ell}$.

capsulated in the scalar product $q_i x^i$. The quadrupolar term decreases $\propto 1/r^3$ with distance. The moments read

$$q = \int_V \mathrm{d}V'\, \rho(\boldsymbol{r}'), \quad q_i = \int_V \mathrm{d}V'\, \rho(\boldsymbol{r}')\, \gamma_{ai} (x')^a, \tag{B.117}$$

and

$$q_{ij} = \int_V \mathrm{d}V'\, \rho(\boldsymbol{r}') \left(\gamma_{ai} (x')^a \gamma_{bj} (x')^b - \frac{r'^2}{3} \gamma_{ij} \right) \tag{B.118}$$

The typical scaling of the potential Φ proportional to $1/r$ for the monopole, $1/r^2$ for the dipole and $1/r^3$ for the quadrupole is illustrated in Fig. 5 for the example of the tetrahedron. Any flat section of $\Phi \times r^{1+\ell}$ as a function of r indicates exactly the behaviour $\Phi \propto 1/r^{1+\ell}$. If there are four positive charges in the corners of the tetrahedron, one sees a dominating Coulomb-potential at large distances, while at shorter distances there is a dipole and a quadrupole contribution. If there are two positive and two negative charges, however, the total charge is zero and there can not be a Coulomb-type contribution to the potential: In fact there is no section with a flat $\Phi \times r$ as a function of r in this case. There is, however, a dominating dipole potential for large radii, and a quadrupolar contribution at small distances.

And additionally, this new definition of the quadrupole moment is traceless,

$$q^i{}_i = \gamma^{ij} q_{ij} = \int_V \mathrm{d}V'\, \rho(\boldsymbol{r}) \left(3 \gamma_{ai} (x')^a \gamma_{jb} (x')^b - r'^2 \gamma_{ij} \right) \gamma^{ij} = 0 \tag{B.119}$$

such that the Cartesian quadrupole moment q_{ij}, as a symmetric, traceless tensor in 3 dimensions has 5 instead of 6 degrees of freedom, commensurate with $q_{\ell m}$ for $\ell = 2$ in spherical coordinates.

B.6 *Potential energy of a charge distribution in a potential*

The same result, perhaps with a bit more physical insight, can be reached by considering the interaction between a charge distribution ρ and an external field Φ. The associated energy W is given by

$$W_{el} = \frac{1}{2}\int_V dV\ \rho(\boldsymbol{r})\Phi(\boldsymbol{r}) \tag{B.120}$$

where ρ acts now as a test charge distribution situated at $\boldsymbol{r} = 0$ in a potential Φ that gets Taylor-expanded around $\boldsymbol{r} = 0$:

$$\Phi(\boldsymbol{r}) = \Phi(\boldsymbol{r})\Big|_{\boldsymbol{r}=0} + \partial_i\Phi\Big|_{\boldsymbol{r}=0} x^i + \frac{1}{2!}\partial_i\partial_j\Phi\Big|_{\boldsymbol{r}=0} x^i x^j \tag{B.121}$$

But for keeping the distinction between test charge and external potential we need to make sure that Φ is not actually sourced by ρ itself: The Poisson-equation would stipulate that

$$\Delta\Phi = -4\pi\rho \tag{B.122}$$

and because the Laplace-operator acting on Φ is identical to the trace of the tensor of second derivatives of Φ, $\gamma^{ij}\partial_i\partial_j\Phi = \Delta\Phi$, it should not be contained in W. Therefore, one defines a traceless tensor

$$\partial_i\partial_j\Phi \quad \rightarrow \quad \partial_i\partial_j\Phi - \frac{\Delta\Phi}{3}\gamma_{ij} \tag{B.123}$$

by subtracting out the trace $\Delta\Phi$, such that the potential becomes

$$\Phi(\boldsymbol{r}) = \Phi(\boldsymbol{r})\Big|_{\boldsymbol{r}=0} + \partial_i\Phi\Big|_{\boldsymbol{r}=0} x^i + \frac{1}{6}\partial_i\partial_j\Phi\Big|_{\boldsymbol{r}=0}\left(3x^i x^j - r^2\gamma^{ij}\right). \tag{B.124}$$

Inclusion of the $r^2\gamma^{ij}$-term does not make any difference, because

$$x^i x^j\left(\partial_i\partial_j\Phi - \frac{\Delta\Phi}{3}\gamma_{ij}\right) = x^i x^j\partial_i\partial_j\Phi - \frac{\Delta\Phi}{3}\underbrace{\gamma_{ij}x^i x^j}_{=r^2} = x^i x^j\partial_i\partial_j\Phi \quad \text{as} \quad \Delta\Phi = 0. \tag{B.125}$$

The definitions of total charge q, dipole moment q^i and quadrupole moment q^{ij} are then identical to those discussed before, and the final expression of the interaction energy would be

$$W_{el} = \frac{1}{2}\int_V dV\ \rho(\boldsymbol{r})\Phi(\boldsymbol{r}) \simeq \frac{1}{2}q\Phi(\boldsymbol{r}) + \frac{1}{2}q^i\partial_i\Phi + \frac{1}{12}q^{ij}\partial_i\partial_j\Phi \tag{B.126}$$

with the interpretation that the interaction energy of nth order multipoles of the charge distribution is sensitive to the nth derivatives of Φ, and that they depend on the magnitude and relative orientation of the eigensystems of the tensors. This point of view is genuinely new, because the energy W can be changed by reorienting the

charge distribution, in addition to displacing it. Additionally, the nth derivatives of the potential become measurable through their interaction energy with a multipole of order n, separate by order.

B.7 *Magnetic vector potential and gauging*

Magnetostatic problems, i.e. the computation of the magnetic fields for a given current density j^i with no contribution from time-varying electric fields require the solution of the fourth Maxwell-equation

$$\epsilon^{ijk}\partial_k \mathrm{H}_k = \frac{4\pi}{c} j^i, \tag{B.127}$$

where this solution needs to fulfill the second Maxwell-equation $\partial_i \mathrm{B}^i = 0$ as a constraint. This constraint would be automatically fulfilled if B^i is derived from a magnetic potential A_i according to $\mathrm{B}^i = \epsilon^{ijk}\partial_j \mathrm{A}_k$, because $\partial_i \mathrm{B}^i = \epsilon^{ijk}\partial_i\partial_j \mathrm{A}_k = 0$, again through contraction of an antisymmetric with a symmetric object. Introducing the constitutive relation $\mathrm{H}_i = \mu_{ij}\mathrm{B}^j$ brings the fourth Maxwell-equation into the form

$$\epsilon^{ijk}\partial_j \mathrm{H}_k = \mu_{kl}\epsilon^{ijk}\partial_j \mathrm{B}^l = \mu_{kl}\epsilon^{ijk}\epsilon^{lmn}\partial_j\partial_m \mathrm{A}_n \tag{B.128}$$

which, for isotropic media with $\mu_{kl} = \gamma_{kl}/\mu$ leads to the Grassmann-relation

$$= \frac{1}{\mu}\left(\gamma^{im}\gamma^{jn} - \gamma^{in}\gamma^{jm}\right)\partial_j\partial_m \mathrm{A}_n = \frac{1}{\mu}\left(\gamma^{im}\partial_m(\gamma^{jn}\partial_j \mathrm{A}_n) - \gamma^{in}(\gamma^{jm}\partial_j\partial_m \mathrm{A}_n)\right). \tag{B.129}$$

⚠ *In an anisotropic medium, the Grassmann-algebra would read* $\mu_{kl}\epsilon^{ijk}\epsilon^{lmn} = \mu^{im}\mu^{jn} - \mu^{in}\mu^{jm}$

There exists the possibility to set the divergence $\gamma^{jn}\partial_j \mathrm{A}_n = 0$, called the Coulomb-gauge, showing that in fact a Poisson-type equation relates A_i and j^i:

⚠ *The Coulomb-gauge in a medium would be* $\mu^{jn}\partial_j \mathrm{A}_n = 0$*...*

$$\Delta \mathrm{A}_i = -\frac{4\pi\mu}{c}\gamma_{ij} j^j, \tag{B.130}$$

after multiplication of the equation with the inverse metric. Perhaps this is the right moment to emphasise that the "vector" potential A_i is in fact a linear form, and that the metric γ_{ij} is needed to convert the vector j^i to a linear form, to make the Poisson-equation notationally consistent.

⚠ *...and the field equation* $\Delta \mathrm{A}_i = -4\pi\mu_{ij} j^j/c$ *with* $\Delta = \mu^{ij}\partial_i\partial_j$

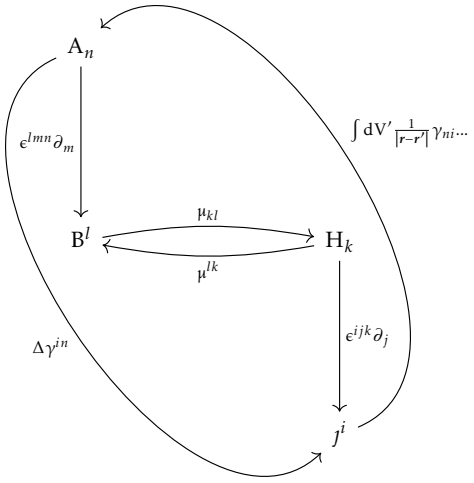
To illustrate the power of a gauge-assumption one could write eqn. (B.129) in matrix-vector notation, for the case of an isotropic medium and brushing slightly over the differences between vectors and linear forms, by using $\mathrm{A}^i = \gamma^{ij}\mathrm{A}_j$ as a vector,

$$\begin{pmatrix} \Delta & 0 & 0 \\ 0 & \Delta & 0 \\ 0 & 0 & \Delta \end{pmatrix} \cdot \begin{pmatrix} \mathrm{A}_x \\ \mathrm{A}_y \\ \mathrm{A}_z \end{pmatrix} - \begin{pmatrix} \partial_x\partial_x & \partial_x\partial_y & \partial_x\partial_z \\ \partial_y\partial_x & \partial_y\partial_y & \partial_y\partial_z \\ \partial_z\partial_x & \partial_z\partial_y & \partial_z\partial_z \end{pmatrix} \cdot \begin{pmatrix} \mathrm{A}_x \\ \mathrm{A}_y \\ \mathrm{A}_z \end{pmatrix} = -\frac{4\pi\mu}{c}\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix}. \tag{B.131}$$

While the first term, where A_i gets multiplied with a diagonal matrix that contains the Laplace-operator Δ, defines a one-to-one mapping of each component of A_i to its corresponding source j^i, the association is broken by the second term, which is non-diagonal and supplies all kinds of mixed derivatives. But the assumption Coulomb-gauge makes these contributions vanish.

The assumption of Coulomb-gauge $\gamma^{jn}\partial_j \mathrm{A}_n = 0$ provides an astounding sim-

plifaction, as each entry of A_i is sourced from each corresponding entry of j^i in three independent Poisson-equations. Without Coulomb-gauge, the term $\partial_i(\gamma^{jn}\partial_j A_n)$ would, as the gradient in the i-direction of the divergence of $\mathbf{A}$, couple all three equations. The interplay between the magnetic potential A_i (in Coulomb-gauge), the magnetic fields H_i, B^i and the source j^i is summarised by this diagram,



(B.132)

The physically measurable magnetic field B^i does not change under ✓ gauge transforms

$$A_i \to A_i + \partial_i \chi \tag{B.133}$$

because

$$B^i = \epsilon^{ijk}\partial_j A_k \to \epsilon^{ijk}\partial_j(A_k + \partial_k\chi) = \epsilon^{ijk}\partial_j A_k + \underbrace{\epsilon^{ijk}\partial_j\partial_k\chi}_{=0} = B^i \tag{B.134}$$

using that the gradient of a scalar field is always curl-free, $\epsilon^{ijk}\partial_j\partial_k$ vanishes as a contraction between an antisymmetric and symmetric tensor. This implies that the potential is only determined up to the gradient $\partial_i\chi$ of a scalar field χ (the gauge field). A particularly constructed field $\partial_i\chi$ can always be added onto A_i for computational convenience, without ever changing the actually measurable field B^i. This convenience might be the assumption of a ✓ gauge condition, for instance $\gamma^{ij}\partial_i A_j = 0$ (called Coulomb-gauge), which is necessary to have Poisson-type potential problems in magnetostatics.

The Coulomb-gauge condition transforms as

$$\gamma^{ij}\partial_i \mathrm{A}_j = 0 \rightarrow \gamma^{ij}\partial_i(\mathrm{A}_j + \partial_j\chi) = \gamma^{ij}\partial_i \mathrm{A}_j + \underbrace{\gamma^{ij}\partial_i\partial_j}_{=\Delta}\chi = 0. \tag{B.135}$$

If the vector potential A_i should be free of any divergence, one can construct χ as a solution to the Poisson-type equation

$$\Delta\chi = -\gamma^{ij}\partial_i \mathrm{A}_j, \tag{B.136}$$

effectively sourcing the gauge function χ with the yet nonzero divergence of the vector potential. It has, due to the Green-theorems, always a unique solution. Applying the gauge-transformation with this gauge field χ effectively cleans up the vector potential and makes it perfectly divergence-free. We can always assume that this has already been taken care of, just by writing $\gamma^{ij}\partial_i \mathrm{A}_j = 0$.