3 Mathematics of the Poisson Equation

3.1 Green functions and the Poisson equation

(a) The Dirichlet Green function satisfies the Poisson equation with delta-function charge

$$-\nabla^2 G_D(\boldsymbol{r}, \boldsymbol{r}_o) = \delta^3(\boldsymbol{r} - \boldsymbol{r}_o) \tag{3.1}$$

and vanishes on the boundary. *It is the potential at $\boldsymbol{r}$ due to a point charge (with unit charge) at $\boldsymbol{r}_o$ in the presence of grounded ($\Phi = 0$) boundaries* The simplest free space green function is just the point charge solution

$$G_o = \frac{1}{4\pi|\boldsymbol{r} - \boldsymbol{r}_o|} \tag{3.2}$$

In two dimensions the Green function is

$$G_o = \frac{-1}{2\pi} \log|\boldsymbol{r} - \boldsymbol{r}_o| \tag{3.3}$$

which is the potential from a line of charge with charge density $\lambda = 1$

(b) The Poisson equation or the boundary value problem of the Laplace equation can be solved once the Dirichlet Green function is known.

$$\Phi(\boldsymbol{r}) = \int_V \mathrm{d}^3 x_o \, G_D(\boldsymbol{r}, \boldsymbol{r}_o)\rho(\boldsymbol{r}_o) - \int_{\partial V} dS_o \, \boldsymbol{n}_o \cdot \nabla_{r_o} G_D(\boldsymbol{r}, \boldsymbol{r}_o)\Phi(r_o) \tag{3.4}$$

where $\boldsymbol{n}_o$ is the *outward* directed normal. The first term is a volume integral and is the contribution of the interior charges on the potential. The second term is a surface integral, and is the contribution of the boundary value to the interior.

(c) A useful technique to find a Green function is image charges. You should know the image charge green functions

i) A plane in 1D and 2D (class)

ii) A sphere (homework)

iii) A cylinder (homework + recitation)

(d) The Green function can always be written in the form

$$G(\boldsymbol{r}, \boldsymbol{r}_o) = \underbrace{G_o(\boldsymbol{r}, \boldsymbol{r}_o)}_{\frac{1}{4\pi|\boldsymbol{r} - \boldsymbol{r}_o|}} + \Phi_{\mathrm{ind}}(\boldsymbol{r}, \boldsymbol{r}_o) \tag{3.5}$$

where the induced potential, $\Phi_{\mathrm{ind}}(\boldsymbol{r}, \boldsymbol{r}_o)$, is regular and satisfies the homogeneous equation $-\nabla^2 \Phi_{\mathrm{ind}} = 0$.

The interaction energy of a point charge q and the grounded boundaries (*i.e.* between the charge q and the induced charges on the grounded surfaces) is entirely due to the induced potential [1]

$$U_{\rm int}(r_o) = q(q\Phi_{\rm ind}(\boldsymbol{r}_o, \boldsymbol{r}_o)) = q^2 \lim_{\boldsymbol{r}\to\boldsymbol{r}_o} \left(G(\boldsymbol{r}, \boldsymbol{r}_o) - G_{\rm o}(\boldsymbol{r}, \boldsymbol{r}_o)\right) \tag{3.6}$$

and the force

$$\boldsymbol{F} = -\nabla_{\boldsymbol{r}_o} U_{\rm int}(\boldsymbol{r}_o) \tag{3.7}$$

(e) Finding the Green function by separation of variables This is best illustrated by example. Pick two dimensions of a surface (say θ, ϕ). The method is motivated by the fact that $\delta^3(\boldsymbol{r} - \boldsymbol{r}_o)$ can be written as a sum

$$\delta^3(\boldsymbol{r} - \boldsymbol{r}_o) = \frac{1}{r^2}\delta(r - r_o)\delta(\cos\theta - \cos\theta_o)\delta(\phi - \phi_o) = \frac{1}{r^2}\delta(r - r_o)\sum_{\ell m} Y_{\ell m}(\theta, \phi)Y^*_{\ell m}(\theta_o, \phi_o) \tag{3.8}$$

Thus the green function is can also be written as

$$G(\boldsymbol{r}, \boldsymbol{r}_o) = \sum_{\ell=0}^{\infty}\sum_{-\ell}^{\ell} g_{\ell m}(r, r_o)Y_{\ell m}(\theta, \phi)Y^*_{\ell m}(\theta_o, \phi_o) \tag{3.9}$$

leading to an equation for $g_{\ell m}(r, r_o)$

$$\left[-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\ell(\ell+1)}{r^2}\right] g_{\ell m}(r, r_o) = \frac{1}{r^2}\delta(r - r_o) \tag{3.10}$$

This remaining equation in 1D is then solved for the green function following the strategy outlined in Sect. 3.2 (see Eq. (3.32)). This depends on the conditions boundary conditions. Similar expressions can be derived in other coordinates.

(f) For free space, the two solutions to Eq. (3.10) are $y_{out}(r) = 1/r^{\ell+1}$ and $y_{\rm in}(r) = r^\ell$, $p(r) = r^2$ and $p(r)W(r) = 2\ell + 1$. Then the free space Green fcn can be written

$$\frac{1}{4\pi|\boldsymbol{r} - \boldsymbol{r}_o|} = \sum_{\ell=0}^{\infty}\sum_{-\ell}^{\ell}\left[Y_{\ell m}(\theta, \phi)Y^*_{\ell m}(\theta_o, \phi_o)\right]\frac{1}{2\ell+1}\frac{r_<^\ell}{r_>^{\ell+1}} \tag{3.11}$$

Some useful identities can be derived from Eq. (3.11):

i) The generating function of Legendre Polynomials is found by setting $\boldsymbol{r}_o = \hat{\boldsymbol{z}}$ and $r < 1$ with $Y_{\ell 0} = \sqrt{(2\ell+1)/4\pi}P_\ell(\cos\theta)$

$$\frac{1}{\sqrt{1 + r^2 - 2r\cos\theta}} = \sum_{\ell=0}^{\infty} r^\ell P_\ell(\cos\theta) \tag{3.12}$$

ii) The spherical harmonic addition theorem which we find by writing by setting $\boldsymbol{r}_o = 1$ and $r < 1$ and using $1/|\boldsymbol{r} - \boldsymbol{r}_o| = 1/\sqrt{1 + r^2 - 2r\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}_o}$

$$P_\ell(\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}_o) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta, \phi)Y^*_{\ell m}(\theta_o\phi_o) \tag{3.13}$$

where $\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}_o$ is the cosine of the angle between the two vectors.

[1] We have multiply by q^2 since the green function is the potential for a unit charge $q = 1$. The electro-static potential for charge q is $qG(\boldsymbol{r}, \boldsymbol{r}_o)$, while the interaction energy is $U = q\Phi_{\rm ind}(\boldsymbol{r}_o, \boldsymbol{r}_o)$.

iii) The shell structure relation which you find by setting $\hat{\boldsymbol{r}} = \hat{\boldsymbol{r}}_o$

$$1 = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta,\phi) Y^*_{\ell m}(\theta,\phi) \tag{3.14}$$

This relation is what is responsible for shell structure in the periodic table

(g) Similar expansion exists in other coordinates. *e.g.* in cylindrical coords $y_{out}(\rho) = K_m(\kappa\rho)$ and $y_{in}(\rho) = I_m(\kappa\rho)$, leading to

$$\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}_o|} = \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} \int \frac{dk}{2\pi} \left[e^{im(\phi-\phi_o)} e^{ik(z-z_o)} \right] I_m(k\rho_<) K_m(k\rho_>) \tag{3.15}$$

3.2 Solving the Laplace Equation by Separation

A summary of separation of variables in different coordinate systems is given in Appendix D. The most important case is spherical and cartesian coordinates.

Solving the Laplace equation

We use a technique of separation of variables in different coordinate systems. The technique of separation of variables is best illustrated by example. For instance consider a potential in a square geometry. The

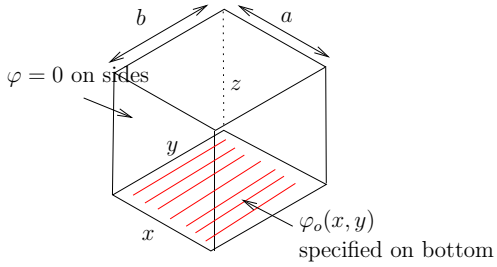

Figure 3.1: A rectangle illustrating separation of vars

potential $\Phi(x,y,z)$ is specified at $z=0$ to be $\Phi_o(x,y)$ and zero on the remaining boundaries

(a) We look for solutions of the separated form

$$\Phi = \underbrace{Z(z)}_{\perp \text{ to surf}} \quad \underbrace{X(x)Y(y)}_{\parallel \text{ to surf}} \tag{3.16}$$

Substituting this into the laplace equation, and separating variables gives two equations for X, Y (the parallel directions)

$$\left[-\frac{d^2}{dx^2} - k_n^2 \right] X(x) = 0\,, \tag{3.17}$$

$$\left[-\frac{d^2}{dy^2} - k_m^2 \right] Y(x) = 0\,. \tag{3.18}$$

and one equation for the perpendicular equation

$$\left[-\frac{d^2}{dz^2} + k_z^2 \right] Z(z) = 0\,, \tag{3.19}$$

where $k_z^2 = k_n^2 + k_m^2$. The signs of k_x, k_y, k_z are chosen for later convenience, because it will be impossible to satisfy the BC for $k_x^2 < 0$ or $k_y^2 < 0$.

The first step is always to separate variables and write down the general solutions to the separated equations

$$X(x) = A\cos(k_n x) + B\sin(k_n x) \tag{3.20}$$
$$Y(y) = A\cos(k_m y) + B\sin(k_m y) \tag{3.21}$$
$$Z(z) = Ae^{-k_z z} + Be^{k_z z} \tag{3.22}$$

(b) It is best to analyze the parallel equations first which are all of the form of a Sturm Louiville *eigenvalue* equation (see below). These determine the (eigen) functions $X(x), Y(y)$ *and* the eigenvalues (or separation constants) k_x and k_y.

The general solution for $X(x)$ is

$$X(x) = A\cos k_x x + B\sin k_x x\,, \tag{3.23}$$

and we are specifying boundary conditions at $x = 0$ and $x = a$. In order to satisfy the boundary condition $X(0) = X(a) = 0$, we must have $A = 0$ and $k = n\pi/a$, leading to

$$X(x) = B\sin(k_n a) \qquad k_n = \frac{n\pi}{a} \quad n = 1, 2, \ldots\,. \tag{3.24}$$

Similarly

$$Y(y) = B\sin(k_m a) \qquad k_m = \frac{m\pi}{a} \quad m = 1, 2, \ldots \tag{3.25}$$

Thus the parallel directions determine both the functions and the separation constants. The complete eigen functions are

$$\psi_{nm}(x, y) = \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right) \qquad n = 1\ldots\infty \qquad m = 1\ldots\infty$$

(c) Finally we return to the perpendicular direction, Eq. (3.19). This equation does not usually constrain the separation constants. The general solution is

$$Z(z) = Ae^{k_z z} + Be^{-k_z z} \tag{3.26}$$

with $k_z = \sqrt{k_n^2 + k_m^2}$. With $Z(z)$ specified The general solution then is a linear combination

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\left[A_{nm}e^{-\gamma_{nm}z} + B_{nm}e^{+\gamma_{nm}z}\right]\psi_{nm}(x, y) \tag{3.27}$$

Solving the separated equations:

After separating variables, *all* of the equations we wil study can be written in Sturm Louiville form:

$$\left[\frac{-d}{dx}p(x)\frac{d}{dx} + q(x)\right]y(x) = \lambda r(x)y(x) \tag{3.28}$$

where $p(x)$ and $r(x)$ are postive definite fcns. Here we record some general properties of these equations.

(a) Given two independent solutions to the differential equation $y_1(x)$ a and $y_2(x)$ The wronskian times $p(x)$ is constant.

$$p(x)\underbrace{\left[y_1(x)y_2'(x) - y_2(x)y_1'(x)\right]}_{\text{wronskian(x)}} = const \tag{3.29}$$

This usually amounts to a statement of Gauss Law.

(b) If boundary conditions are specified at two endpoints, $x = a$ and $x = b$, then the problem becomes an *eigenvalue* equation.

In this case only certain values of $\lambda = \lambda_n$ are allowed and the functions are uniquely determined up to normalization

$$\left[\frac{-d}{dx}p(x)\frac{d}{dx} + q(x)\right]\psi_n(x) = \lambda_n r(x)\psi_n(x) \tag{3.30}$$

The parallel equations will have this form (see Eq. (3.17)), and notice how the boundary conditions at $x = 0$ and $x = a$ fixed the value of k_n (see Eq. (3.23) and Eq. (3.24)).

The resulting eigenfunctions are complete [2] and orthogonal with respect to the weight $r(x)$

$$\int_a^b dx\, r(x)\psi_n^*(x)\psi_m(x) = 0 \qquad n \neq m \tag{3.31}$$

where a and b are the endpoints where the boundary conditions are specified. Note that the eigenfunctions are complete, only in the space of functions that satisfy the boundary conditions.

(c) **S**olving the separated equations with δ function source terms

We will also need to know the green function of the one dimensional equation

$$\left[\frac{-d}{dx}p(x)\frac{d}{dx} + q(x)\right]g(x, x_o) = \delta(x - x_o) \tag{3.32}$$

The Green function for such 1D equations is based on knowing two homogeneous solutions $y_{out}(x)$ and $y_{in}(x)$, where $y_{out}(x)$ satisfies the boundary conditions for $x > x_o$, and $y_{in}(x)$ satisfies the boundary conditions for $x < x_o$.

The Green function is continuous but has discontinuous derivatives. Since we know the solutions outside and inside it takes the form:

$$G(x, x_o) = C\left[y_{out}(x)y_{in}(x_o)\theta(x - x_o) + y_{in}(x)y_{out}(x_o)\theta(x_o - x)\right] \tag{3.33}$$

$$\equiv C y_{out}(x_>)y_{in}(x_<) \tag{3.34}$$

where C is a constant determined by integrating the equation, Eq. (3.32), across the delta function. In the second line we use the common (but somewhat confusing notation)

$$x_> \equiv \text{the greater of } x \text{ and } x_o \tag{3.35}$$

$$x_< \equiv \text{the smaller of } x \text{ and } x_o \tag{3.36}$$

which makes the second line mean the same as the first line.

Integrating from $x = x_o - \epsilon$ to $x = x_o + \epsilon$ we find the jump condition which enters in many problems:

$$-p(x)\left.\frac{dg}{dx}\right|_{x_o+\epsilon} + p(x)\left.\frac{dg}{dx}\right|_{x_o-\epsilon} = 1\,, \tag{3.37}$$

which can be used to find C.

(d) In fact the jump condition will always involve the Wronskian of the two solutions. Substituting Eq. (3.33) into Eq. (3.37) we see that $C = 1/(p(x_o)W(x_o))$

$$G(x, x_o) = \frac{\left[y_{out}(x)y_{in}(x_o)\theta(x - x_o) + y_{in}(x)y_{out}(x_o)\theta(x_o - x)\right]}{p(x_o)W(x_o)} \tag{3.38}$$

$$\equiv \frac{y_{out}(x_>)y_{in}(x_<)}{p(x_o)W(x_o)} \tag{3.39}$$

where $W(x_o) = y_{out}(x_o)y'_{in}(x_o) - y_{in}(x_o)y'_{out}(x_o)$ is the Wronskian. Note that the denominator $p(x_o)W(x_o)$ is constant and is independent of x_o.

[2] See Morse and Freshbach