18.303 Problem Set 7

Due Wednesday, 26 October 2011.

Problem 1: Green's functions

Consider Green's functions of the positve-definite operator $\hat{A} = -\nabla^2 + \kappa^2$ ($\kappa > 0$) over all space ($\Omega = \mathbb{R}^3$ in 3d), with solutions that $\to 0$ at infinity. As in class, thanks to the translational and rotational invariance of this problem, we can find $G(\mathbf{x}, \mathbf{x}') = g(|\mathbf{x} - \mathbf{x}'|)$ for some $g(r)$ in spherical/cylindrical coordinates.

(a) Solve for $g(r)$ in 3d.

(i) Similar to the case of $\hat{A} = -\nabla^2$ in class, first solve for $g(r)$ for $r > 0$, and write $g(r) = \lim_{\epsilon \to 0^+} f_\epsilon(r)$ where $f_\epsilon(r) = 0$ for $r \le \epsilon$. [Hint: although Wikipedia writes the spherical $\nabla^2 g(r)$ as $\frac{1}{r^2}(r^2 g')'$, it may be more convenient to write it equivalently as $\nabla^2 g = \frac{1}{r}(rg)''$, as in class, and to solve for $h(r) = rg(r)$ first.]

(ii) Then, evaluate $\hat{A}g = \delta(\mathbf{x})$ in the distributional sense: $(\hat{A}g)\{q\} = g\{\hat{A}q\} = q(0)$ for an arbitrary (smooth, localized) test function $q(\mathbf{x})$ to solve for the unknown constants in $g(r)$. [Hint: when evaluating $g\{\hat{A}q\}$, you may need to integrate by parts on the radial-derivative term of $\nabla^2 q$; don't forget the boundary term(s).]

(b) Check that the $\kappa \to 0^+$ limit gives the answer from class.

(I was thinking of assigning the 2d case, but the solution involves a modified Bessel function and seemed a bit much for homework. However, the 2d case with $\kappa = 0$ is quite doable — I assigned it in last year's pset 6, which you can look at online.)

Problem 2: Deltas, derivatives, and limits

(a) Consider the "finite δ" function

$$\delta_{\Delta x}(x) = \frac{1}{(\Delta x)^2} \begin{cases} \Delta x - |x| & |x| < \Delta x \\ 0 & |x| \ge \Delta x \end{cases},$$

which has area = 1 and hence $\lim_{\Delta x \to 0^+} \delta_{\Delta x} = \delta$ ("=" in the sense of distributions, of course). Explicitly evaluate the (distributional) second derivative $\frac{d^2}{dx^2}\delta_{\Delta x}$ (using δ functions as needed). Show that this corresponds to a difference approximation for $\frac{d^2}{dx^2}\delta$, and hence converges to the latter as $\Delta x \to 0$.

(b) In 8.02, you defined a "dipole" as two point charges $+q$ and $-q$ separated by a distance Δx, with "dipole moment" $p = qd$. We can write this (in 1d) as a charge density $\rho(x) = q\delta(x - d/2) - q\delta(x + d/2)$. Show that if we take the limit $d \to 0$ while keeping p fixed (i.e. $q = p/d \to \infty$), that $\rho(x)$ goes to something involving the derivative $\delta'(x)$. [Hint: relate $\rho\{\phi\}$ for finite d to a difference approximation of $\phi'(0)$.]

Problem 3: van der Waals forces

In the class notes on Green's functions in inhomogeneous media, section 3.1, the solution of a "dipole" source $\mathbf{p}$ (e.g. the potential an electrostatic point dipole $\mathbf{p}$) is given as $D_\mathbf{p}(\mathbf{x}, \mathbf{x}') = \mathbf{p} \cdot \nabla' G_0(\mathbf{x}, \mathbf{x}') = \mathbf{p} \cdot \frac{\mathbf{x} - \mathbf{x}'}{4\pi|\mathbf{x} - \mathbf{x}'|^3}$. This is the solution $u_0(\mathbf{x}) = D_\mathbf{p}(\mathbf{x}, \mathbf{x}_0)$ from a point dipole at $\mathbf{x}_0$, i.e. $-\nabla^2 u_0 = -\mathbf{p} \cdot \nabla\delta(\mathbf{x} - \mathbf{x}_0)$.

(a) Suppose that we now place our dipole in a slightly inhomogeneous medium, so that the solution u satisfies $-\nabla \cdot (c\nabla u) = -\mathbf{p} \cdot \nabla\delta(\mathbf{x} - \mathbf{x}_0)$ where $c(\mathbf{x}) = 1$ everywhere except in a small volume V centered at $\mathbf{x}_1$ where c equals c_1 ($|c_1 - 1| \ll 1$), similar to section 3 of the notes. Similar to section 3, derive the new solution $u(\mathbf{x})$ in the first Born approximation. (Hint: there is a quick way to do it, similar to how $D_\mathbf{p}$ was derived.)

(b) In electrostatics, u is the electric potential from a dipole $\mathbf{p}$, and $\mathbf{E} = -\nabla u$ is the electric field. The energy of a dipole in an electric field is $-\mathbf{p} \cdot \mathbf{E} = \mathbf{p} \cdot \nabla u$. The *interaction energy* of the dipole and the inhomogeneity in V is given by $\mathbf{p} \cdot \nabla(u - u_0)$, the energy due to the *change* in the potential from V. Compute this interaction energy in the first Born approximation.

(c) Suppose that $\mathbf{p}$ is randomly fluctuating, e.g. it is a water molecule with an orientation that is rotating randomly in time due to thermal fluctuations, so that the mean $\mathbf{p}$ is zero but the mean $|\mathbf{p}|^2$ is $\neq 0$. Argue from your result in the previous part[1] that there is a nonzero mean interaction energy, and hence a nonzero mean force (from the derivative of the interaction energy with separation $d = |\mathbf{x}_1 - \mathbf{x}_0|$). How does the force scale with d? What is the sign of the force if $c_1 > 1$ [in electrostatics, $c =$ (refractive index)$^2 \geq 1$], attractive or repulsive?

You have just derived (at a very simple level, without worrying about the source of the fluctuations in $\mathbf{p}$) a *van der Waals force*. vdW forces arise in general between neutral particles whose dipole moments are fluctuating (due to thermal or quantum fluctuations) because each dipole's field polarizes the other particle (or "scatters" off of it, in the Born approximation), creating an interaction that scales with distance like the result you (hopefully) just derived.

[1] Technically, to apply your result in the previous part you must make a "quasistatic" approximation: you must assume that the time d/c for light to propagate over the distance $d = |\mathbf{x}_1 - \mathbf{x}_0|$ is much smaller than the time for $\mathbf{p}$ to change, so that we can neglect the finite speed of light and use the static dipole potential. This is true for small d but fails for large d/c relative to a typical fluctuation timescale, and in that regime the usual van der Waals force is replaced by a "Casimir–Polder" force that incorporates the finite speed of light.