Tutorial 2 for MATH4220

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1. Schrodinger Equation

Consider the Hydrogem Atom. This is an electron moving around a proton. Let m be the mass of the electron, e the charge, and h Planck's constant divided by 2π. Let the origin of coordinates (x, y, z) be the position of the proton and let $r = (x^2 + y^2 + z^2)^{\frac{1}{2}}$ be the spherial coordinate.

Let $u(x, y, z, t)$ be the wave function which represents a possible state of the electron, and $|u|^2$ represents the probability density of the electron at position (x, y, z) and time t. If D is any region of the space, then $\iiint_D |u|^2 dxdydz$ is the probability of finding the electron in the region D at time t. Thus

$$\iiint_{\mathbb{R}^n} |u|^2 dxdydz = 1$$

The motion of the electron satisfies Schrodinger equation:

$$-ihu_t = \frac{h^2}{2m}\triangle u + \frac{e^2}{r}u$$

in all of space $-\infty < x, y, z < \infty$

2. Condition at infinity.

When the domain is unbounded, what kind of the condition should we impose? The physics usually provides conditions at infinity.

For example, consider the Schrodinger equation where the domain is the whole space. Since

$$\iiint_{\mathbb{R}^n} |u|^2 dxdydz = 1$$

we know that u "vanishes at infinity", that is,

$$\lim_{r \to +\infty} u(x, y, z, t) = 0$$

where r is the spherical coordinates.

3. Boundary conditions for sound waves.

*Any questions about the notes, please email me at rzhang@math.cuhk.edu.hk

Small disturbances are governed by

$$\begin{aligned} \frac{\partial \mathbf{v}}{dt} + \frac{c_0^2}{\rho_0}\nabla\rho = 0 \\ \frac{\partial \rho}{dt} + \rho_0 \mathrm{div}\mathbf{v} = 0 \end{aligned} \tag{1}$$

where $\mathbf{v}$ and ρ as unknowns are velocity and density. ρ_0 is the density and c_0 is the speed of sound in still air.

Assume that the is no swirl of the sound, that is, curl$\mathbf{v} = 0$. Then (1) can be written as

$$\begin{aligned} \frac{\partial^2 \mathbf{v}}{dt^2} = c_0^2 \Delta \mathbf{v} \\ \frac{\partial^2 \rho}{dt^2} = c_0^2 \Delta \rho_0 \end{aligned} \tag{2}$$

Boundary conditions:

Case 1: $\mathbf{v} \cdot \mathbf{n} = 0$: the sound propagates in a closed sound-insulated room with rigid wall. Furthermore, curl$\mathbf{v} = 0$ implies that there exists a scaler function ϕ such that $v = \nabla\phi$. Thus this boundary condition turns to $\frac{\partial \phi}{\partial \mathbf{n}} = 0$, Neumann boundary conditon for ϕ.

Case 2: $\rho = \rho_0$: at an open window. Dirichlet Boundary condition for ρ.

Case 3: $\mathbf{v} \cdot \mathbf{n} = a(\rho - \rho_0)$: at a soft wall.