QM-18 Lecture Notes
Scattering in Quantum Mechanics*
18.2 Setting up integral equation

A.K. Kapoor
http://0space.org/users/kapoor
akkhcu@gmail.com; kapoor.proofs@gmail.com

Contents

1 A simple example

Setting up integral equation

Very often the problem of solving a linear differential equation can be replaced with solution of an integral equation. An important feature of the integral equation approach is that the initial conditions to be satisfied by the solution is built into the integral equation. The integral equation can be solved many a times by an iterative procedure which we shall illustrate by an example of a simple differential equation.

Suppose we are interested in solving the differential equation

$$\frac{dy}{dx} = \lambda y \tag{1}$$

subject to the boundary condition

$$y(x)|_{x=x_0} = N \tag{2}$$

where N is a constant. To convert Eq.(1) into an integral equation we integrate Eq.(1) to get

$$y(x) = \lambda \int y(x)dx + constant \tag{3}$$

or to be more precise, let us write Eq.(3) as

$$y(x) = \lambda \int_0^x y(t)dt + constant \tag{4}$$

The constant in the above equation is fixed by making use of the initial condition Eq.(2), and we get const= N and

$$y(x) = N + \lambda \int_0^x y(t)dt \tag{5}$$

* KAPOOR //qm-lnu-18001.tex; December 12, 2016

It is to noted that the unknown function y appears inside the integral sign, hence an equation of this type is called integral equation. This equation can be solved iteratively giving a solution as a series in powers of λ. This method gives the exact answer in the case of this simple example under consideration.

Perturbative Solution

As a first step, we set y equal to y_0 where

$$y_0 = N \tag{6}$$

is the solution in the zeroth order in λ and is simply taken to be equal to the first term Eq.(5). Next the zeroth order 'solution' ,y_0, is substituted in the right hand side of Eq.(5) to get the solution in the first order in λ. Thus we have

$$\begin{aligned} y_1(x) &= N + \lambda \int_0^x y_0 dx & (7) \\ &= N + \lambda \int_0^x N dx & (8) \end{aligned}$$

$$\therefore \qquad y_1(x) = N(1+\lambda)x \tag{9}$$

To improve the approximation, we substitute $y_1(x)$ for $y(x)$ in right hand side of Eq.(2) to get the next approximation $y_2(x)$ for our solution.

$$\begin{aligned} y_2(x) &= N + \lambda \int_0^x y_1(x) dx & (10) \\ &= N + \lambda \int_0^x N(1+\lambda x) dx & (11) \\ &= N\left(1 + \lambda x + \lambda^2 \frac{x^2}{2}\right) & (12) \end{aligned}$$

continuing in this fashion we get

$$\begin{aligned} y_3(x) &= N + \lambda \int_0^x y_2(x) dx & (13) \\ &= N + N\lambda \int_0^x \left(1 + \lambda x + \lambda \frac{x^2}{2}\right) dx & (14) \\ &= N\left(1 + \lambda x + \frac{\lambda^2 x^2}{2} + \frac{\lambda^3 x^3}{3!}\right) & (15) \\ y_4(x) &= N\left(1 + \lambda x + \frac{\lambda^2 x^2}{2} + \frac{\lambda^3 x^3}{3!} + \frac{\lambda^4 x^4}{4!}\right) & (16) \end{aligned}$$

Thus we get an infinite series in powers of λ

$$y(x) = N\left(1 + \lambda x + \frac{\lambda^2 x^2}{2} + \frac{\lambda^3 x^3}{3!} + \ldots\right) \tag{17}$$

summing the series we get

$$y(x) = Ne^{\lambda x} \tag{18}$$

Note that this is the correct solution for ordinary differential equation and satisfies the given boundary condition $y(0) = N$.

Alternate approach – Using series expansion

The above method of solution is equivalent to the following alternate sequence of steps. We want to solve

$$y(x) = N + \lambda \int_0^x y(t) dt \tag{19}$$

we assume that the solution can be written as a series in λ

$$y(x) = \alpha_0 + \lambda\alpha + \lambda^2\alpha^2 + \cdots + \alpha^n\lambda^n + \cdots \tag{20}$$

we substitute Eq.(20) in Eq.(19) and compare powers on both the sides. Therefore we get

$$\alpha_0(x) + \lambda\alpha_1(x) + \lambda^2\alpha_2(x) + \ldots \lambda^n\alpha_n(x) + \ldots \tag{21}$$
$$= N + \lambda \int_0^x \{\alpha_0(t) + \lambda\alpha_1(t) + \lambda^2(t)\alpha_2(t) + \cdots\} \, dt \tag{22}$$

on comparing coefficients of different powers of λ we successively get

$$\begin{aligned}
\alpha_0(x) &= N \\
\alpha_1(x) &= \int_0^x \alpha_0(t)dt = Nx \\
\alpha_2(x) &= \int_0^x \alpha_1(t)dt = N\frac{x^2}{2} \\
\alpha_1(x) &= \int_0^x \alpha_2(t)dt = N\frac{x^3}{3!} \\
\alpha_k(x) &= \int_0^x \alpha_{k-1}(t)dt = N\frac{x^k}{k!} \qquad (23)
\end{aligned}$$

Therefore we get

$$y(x) = N\left(1 + \lambda x + \frac{\lambda^2}{2!}x^2 + \cdots + \frac{\lambda^n}{n!}x^n + \cdots\right) \tag{24}$$

2 Green function for Poisson equation

In electromagnetic theory the electric potential satisfies the Poisson equation

$$\nabla^2\Phi = -\frac{\rho}{\varepsilon_0}, \tag{25}$$

where $\rho(\vec{r})$ is the volume charge density. The Green function for the Poisson equation is defined by

$$\nabla^2 G(\vec{r}) = -\delta^3(\vec{r}) \tag{26}$$

If $\phi_0(\vec{r})$ is a solution of the Laplace equation

$$\nabla^2\phi_0(\vec{r}) = 0, \tag{27}$$

then

$$\Phi(\vec{r}) = \phi_0(\vec{r}) + \int G(\vec{r} - \vec{r}')\frac{\rho(\vec{r}')}{\varepsilon_0}d^3r' \tag{28}$$

is a solution of the Poisson equation which can be easily verified by applying ∇^2 on both sides of Eq.(28).

$$\begin{aligned}
\nabla^2\Phi(\vec{r}) &= \nabla^2\phi_0(\vec{r}) + \nabla^2 \int G(\vec{r} - \vec{r}')\frac{\rho(\vec{r}')}{\varepsilon_0}d^3r' \qquad (29) \\
&= \int \nabla^2 G(\vec{r} - \vec{r}')\frac{\rho(\vec{r}')}{\varepsilon_0}d^3r' \qquad (30) \\
&= -\frac{1}{\varepsilon_0}\int \delta^3(\vec{r} - \vec{r}')\rho(\vec{r}')d^3\vec{r}' \qquad (31) \\
&= -\frac{\rho(\vec{r})}{\varepsilon_0} \qquad (32)
\end{aligned}$$

It can be shown that one solution of Eq.(26) is

$$G(\vec{r}) = \frac{1}{4\pi r}. \tag{33}$$

This Green function gives the potential due to a charge distribution subject to the condition that the potential vanishes at infinity. The exact form of the Green function and the solution ϕ_0 of the Laplace equation is determined by the boundary conditions of the problem.

3 Integral Equation for Scattering

In order to convert the Schrodinger equation

$$\left\{\frac{-\hbar^2}{2\mu}\nabla^2 + v(r)\right\}\psi = E\psi \tag{34}$$

into an integral equation we first rewrite it as

$$\left(\nabla^2 + k^2\right)\psi = u(\vec{r})\psi(\vec{r}) \tag{35}$$

where $k^2 = \dfrac{2\mu E}{\hbar^2}$, $U(r) = \dfrac{2\mu}{\hbar^2}V(r)$ and we have defined Green function $G(\vec{r})$ as a solution of

$$\left(\nabla^2 + k^2\right)G(\vec{r}) = -\delta(\vec{r}) \tag{36}$$

and it was found that several solutions of Eq.(36) exist.Thus $G(\overrightarrow{r})$ can

$$G_{\pm}(\vec{r}) = \frac{1}{4\pi r}\exp \pm kr \tag{37}$$

$$G_0(\vec{r}) = \frac{1}{4\pi r}\cos(kr) \tag{38}$$

using the Green function we shall now write down a ”formal” solution of Eq.(35) as a solution of integral equation. Next we shall determine the behaviour of the solution as $r \to \infty$ and show that the choice

$$G(\vec{r}) = \frac{1}{4\pi r}\exp ikr \tag{39}$$

leads to the correct boundary condition on the wave function. Using a Green function which is a solution of Eq.(36) a formal solution for Eq.(35) can be written as

$$\psi(\vec{r}) = \phi(\vec{r}) - \int G(|\vec{r}-\vec{r}\,'|)U(|\vec{r}\,'|)\psi(\vec{r}\,')d^3r' \tag{40}$$

where $\phi(\vec{r})$ is a solution of the equation

$$\left(\nabla^2 + k^2\right)\phi(\vec{r}) = 0 \tag{41}$$

For the scattering problem we must select

$$\phi(\vec{r}) = \exp(i\vec{k_i}.\vec{r}) \tag{42}$$

where $\vec{k_i}$ is the momentum of the incident particles.Substituting Eq.(39) Eq.(42) in Eq.(40) we get the integral equation for the scattering to be

$$\psi(\vec{r}) = \exp(i\vec{k_i}.\vec{r}) - \frac{1}{4\pi}\int \frac{\exp^{ik|\vec{r}-\vec{r'}|}}{|\vec{r}-\vec{r'}|}U(\vec{r'})\psi(\vec{r'})d^3r\prime \tag{43}$$

To verify that $\psi(\vec{r})$ given by Eq.(43) does indeed have correct asymptotic property we expand $|\vec{r}-\vec{r'}|$ in powers of $\dfrac{\vec{r}}{\vec{r'}}$ we shall assume that the potential is short range potential so that the contribution to integral over $\vec{r'}$ comes from small value of r'. Expand $|\vec{r}-\vec{r'}|$ in powers of r'

$$|\vec{r}-\vec{r'}| = \sqrt{r^2 + r'^2 - 2\vec{r}\cdot\vec{r'}} \tag{44}$$

$$= r\left(1 - 2\frac{\vec{r}\cdot\vec{r'}}{r^2} + \frac{r'^2}{r^2}\right)^{1/2} \tag{45}$$

Using binomial expansion we get

$$|\vec{r}-\vec{r'}| = r\left(1 - \frac{\vec{r}\cdot\vec{r'}}{r^2} + O\left(\frac{r'^2}{r^2}\right)^2\right) \tag{46}$$

We substitute Eq.(46) in the exponential and in the factor $\dfrac{1}{|\vec{r}-\vec{r'}|}$ in Eq.(43) and write $\dfrac{1}{|\vec{r}-\vec{r'}|} \approx \dfrac{1}{r}$ to get

$$\psi(\vec{r}) \longrightarrow \exp(i\vec{k_i}\cdot\vec{r}) - \frac{1}{4\pi r}\int \exp\left(ikr - ik\frac{\vec{r}\cdot\vec{r'}}{r^2}\right)U(\vec{r'})\psi(\vec{r'})d^3r' \tag{47}$$

$$= \exp(i\vec{k_i}\cdot\vec{r}) - \frac{e^{ikr}}{4\pi r}\int \exp(-ik\hat{n}\cdot\vec{r'})U(r')\psi(r')d^3r' \tag{48}$$

In the last step we have introduced a unit vector $\hat{n} = \vec{r}/r$. The Eq.(48) gives the probability amplitude (wave function) at $\vec{r}$. If the particles are to reach at a detector at $\vec{r}$, the vector $\hat{n}$ must be in the direction of the final momentum and parallel to k_f. Note that

$$|\vec{k}_i| = |\vec{k}_f| = k \tag{49}$$

holds as a consequence of energy conservation and hence

$$k(\hat{n}\cdot\vec{r}') = \vec{k}_f\cdot\vec{r} \tag{50}$$

Thus Eq.(48) takes the form

$$\psi(\vec{r}) \approx \exp(i\vec{k}_i\cdot\vec{r}) - \frac{e^{ikr}}{4\pi r}\int \exp(-i\vec{k}\cdot\vec{r}')U(r')\psi(r')d^3r' \tag{51}$$

This asymptotic behaviour is of the for expected for large r

$$\psi(\vec{r}) \approx \exp(i\vec{k}_i\cdot\vec{r}) - \frac{e^{ikr}}{r}f(\theta,\phi). \tag{52}$$

Comparing Eq.(51) with Eq.(52) we see that the scattering amplitude is given by

$$\begin{aligned} f(\theta,\phi) &= -\frac{1}{4\pi}\int \exp(-i\vec{k}_f\cdot\vec{r}')U(r')\psi(r')d^3r' && (53)\\ &= -\left(\frac{\mu}{2\pi\hbar^2}\right)\int \exp(-i\vec{k}_f\cdot\vec{r}')V(r')\psi(r')d^3r' && (54)\end{aligned}$$

It must be noted that the integral equation Eq.(43) and the expression for the scattering amplitude in Eq.(54) are **exact** results. We shall next discuss how to use (43) and (54) to obtain scattering amplitude in the Born approximation.