Notes for Lecture 18

Born approximation

In the last lecture, we studied a partial wave view of the scattering problem. Concepts such as the optical theorem, the shadow scattering, and the scattering length are some of the important concepts that can be explained naturally from such a view.

Here, we turn to another common way to treat a scattering problem. The new method – the Born approximation – is complimentary to the method of partial waves. It can deal with the case when the potential energy is small, regardless of the magnitude of k. On the other hand, the method of partial waves is the main method to use if the probe beam has low energy – then the low angular momentum partial wave approximation is good regardless of the strength of the potential.

18.1 Green's function

The Green's function is a fundamental way to "break down" a differential equation, and is of tremendous importance. You have already encountered it in E&M, as we will review now. You may also have encountered it for the "driven oscillator problem" in classical mechanics.

18.1.1 Well-known example – good old Coulomb's law

First of all, a notation warning. For this subsection, ϕ will be used to denote the electrostatic potential. As we did in LN 14. ϕ is *not* the azimuthal angle in the spherical coordinate system! However, in a later section (Section 18.2) of this lecture note, ϕ *will* be used for the azimuthal angle. So, a warning.

We are rather familiar with the Green's function in the electrostatics. Namely, we know that the electric field due to a charge density distribution, $\rho(\vec{r})$, is given by $\phi(\vec{r}) = \int d^3\vec{r}\,'\,\rho(\vec{r}\,')/(4\pi\epsilon_0|\vec{r}-\vec{r}\,'|)$. A proper way to understand this expression is that a small local charge $d^3\vec{r}\,'\,\rho(\vec{r}\,')$ exerts a Coulomb potential $d^3\vec{r}\,'\,\rho(\vec{r}\,')/(4\pi\epsilon_0|\vec{r}-\vec{r}\,'|)$, and the integral symbol $\int$ means just a sum. If this small charge is replaced by a unit charge, which means a delta function charge density since the limit $d^3\vec{r} \to 0$ is automatically implied by the infinitesimal symbol, then what we get is the so-called Green's function in the (non-relativistic) electrostatics.

To summarize, the Green's function for the Poisson equation

$$-\nabla^2\phi = \frac{\rho(\vec{r})}{\epsilon_0} \tag{18.1}$$

is given by

$$G(\vec{r}-\vec{r}\,') = \frac{1}{4\pi\epsilon_0}\cdot\frac{1}{|\vec{r}-\vec{r}\,'|} \qquad \text{a solution if } \rho(\vec{r}) = \delta(\vec{r}-\vec{r}\,') \tag{18.2}$$

That is

$$-\nabla_r^2\,G(\vec{r}-\vec{r}\,') = \frac{\delta(\vec{r}-\vec{r}\,')}{\epsilon_0} \tag{18.3}$$

where ∇_r means the gradient operator for $\vec{r}$. The full solution to the Poisson equation is then simply the convolution of the Green's function and the charge density function

$$\phi(\vec{r}) = \int d^3\vec{r}\,\rho(\vec{r})\,G(\vec{r}-\vec{r}\,') \qquad \text{a particular solution} \tag{18.4}$$

The reason that this works is because of the **linearity** of the above Poisson equation as far as the dependence of the *particular* solution ϕ on charge density is concerned.

What do we mean by this **linearity**? First, consider the right hand side of the above Poisson equation a *source term*. Namely, the source term is $\rho(\vec{r})$ up to a constant factor. Second, consider $\phi(\vec{r})$ as the *response* to the source. The linearity means if multiple sources are placed, then the total response is simply the sum of individual responses.

More formally, the following mathematics summarizes this linearity. Take Eq. 18.3 and convolve the charge density with it by multiplying it with the *integral (= sum) operator* $\int d^3\vec{r}\,'\,\rho(\vec{r}\,')$ from the left. By doing so, we get

$$-\nabla_r^2 \int d^3\vec{r}\,'\,\rho(\vec{r}\,')G(\vec{r}-\vec{r}\,') = \frac{\int d^3\vec{r}\,'\,\rho(\vec{r}\,')\delta(\vec{r}-\vec{r}\,')}{\epsilon_0} = \frac{\rho(\vec{r})}{\epsilon_0}$$

which proves, formally, why Eq. 18.4 is indeed a solution to the original Poisson equation Eq. 18.1.

To succinctly summarize all this, we note that the mathematical identity ("Gauss's law" or "divergence theorem")

$$-\nabla^2\left(\frac{1}{4\pi r}\right) = \nabla\cdot\left(\frac{\vec{e}_r}{4\pi r^2}\right) = \delta(\vec{r}) \tag{18.5}$$

and the linearity of the ∇^2 operator provide the core contents on which all our findings rest.

Of course, the *general* solution to the above Poisson equation is not just a particular solution, but must be written as

$$\phi(\vec{r}) = \phi_h(\vec{r}) + \int d^3\vec{r}\,\rho(\vec{r})\,G(\vec{r}-\vec{r}\,') \tag{18.6}$$

where ϕ_h is the homogeneous solution. That is, ϕ_h satisfies the Laplace equation $\nabla^2\phi_h = 0$. This general solution must be used to find a solution that fits a prescribed boundary condition.

18.1.2 Green's function in quantum mechanics

The subject of Green's function in quantum mechanics is an incredibly deep one, since, in the most general quantum mechanical situation, it, not the wave function, is the most fundamental quantity. This does not mean that it is OK not to know the wave function. It is just that the Green's function takes the front seat, and the wave function takes the back seat. Here, we get a really primitive taste of the Green's function in quantum mechanics, by considering the simple one-particle time-independent Schrödinger equation that we have been considering and loving so far. Hey, this is a great way to start!

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{18.7}$$

$$\left(\nabla^2 + k^2\right)\psi = \frac{2m}{\hbar^2}V\psi \qquad\qquad k \equiv \sqrt{2mE}/\hbar \tag{18.8}$$

Right here, we might feel a bit tingly in our stomach. In this equation, we *can* consider the right hand side as the source term. After all, V is what makes these problems difficult to solve, so that must be the "source of all difficulties." And then, we can consider the wave function ψ as the response to it. But, here is a problem that may make us feel uneasy. We have a circular situation – the source is dependent on ψ (as well as V) to begin with! We have a chicken and egg situation!

At this point, you *could* think "Gee ... this looks to be one of those weird things that tend to happen in quantum mechanics ... I will just hold my nose and somehow get done with it." But do not think this way. Wise students here in Santa Cruz do not. The correct way to think is the following. "Hmm, interesting ... if this is what quantum mechanics tells me, then it must be that *everything* is like this at a fundamental level ... I must recognize the importance of this type of circular dependence and learn to accept and love it." To make this point clearer, notice that the superficial separation between the source (charge) and the response (potential) in the electrostatic problem above is only a facade. If one considers a two body problem, or a two metallic spheres at different potentials, or any non-trivial closed system electrostatic problem, then one will realize that the relation between the charge and the potential is indeed a circular one, and the only way to solve for them is to find them at the same time!

So, we should not feel too strange, and in fact you should feel *even quite natural*, when we take the right hand side of Eq. 18.8 as a source term, even if it contains the response. Then, what we have is basically a Green's function problem for the Helmholtz equation[1]

$$\left(\nabla^2 + k^2\right) G(\vec{r}) \;=\; \delta(\vec{r}) \qquad\qquad \delta(\vec{r}) \text{ replacing } \frac{2m}{\hbar^2} V\psi \tag{18.9}$$

One could solve this problem like the textbook does, which is a good lesson, since the steps involve some pretty indispensable tools – Fourier transform and Cauchy's residue theorem. I hope you will make yourself very familiar with those mathematical tools, if you are not already. Here, we will solve this problem somewhat differently.

Note first that $G(\vec{r}) = -1/(4\pi r)$ will *almost* do: by Eq. 18.5 it takes care of the $\nabla^2 G = \delta(\vec{r})$ part, but it does not do anything about the k^2 part. A reasonable idea is then

$$G(\vec{r}) \;=\; -\frac{u(r)}{4\pi r} \quad \text{with} \quad u(r \to 0) \;=\; 1 \tag{18.10}$$

Note that this ansatz, with $u(r)$ a regular function, completely takes care of the delta function singularity at the origin. All we need to do then is to find the correct $u(r)$ that makes this a solution of Eq. 18.9 for $r > 0$. If we find such $u(r)$, then $-u(r)/(4\pi r)$ *will* be proved to be a solution.

Now, the form of the wave function $u(r)/r$ is something that we are quite familiar with (radial wave function $R = u/r$). Multiplying the ∇^2 operator on u/r, we get the radial Schrödinger equation (Eq. 17.3) for $u(r)$. Also, note that, the radial equation always concerns $r > 0$ only, *not* including the $r = 0$ point, which is a singular point,

[1]Note that $\delta(\vec{r})$ is sometimes written as $\delta^3(\vec{r})$.

whose singular nature is introduced by the Cartesian to spherical coordinate transformation itself. Noting, then, that $V \propto \delta(\vec{r})/\psi$ is zero for $r > 0$ for the current Green's function problem, the radial equation is simply a free particle problem. This is all good and well for us, since we need to find the solution $u(r)$ will satisfy the above equation for $r > 0$!

Furthermore, we shall assume $l = 0$, for the obvious reason of symmetry, and the fact that our goal is to find *one* particular solution. Thus, the radial equation for the current problem is given by

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = E\,u(r) \tag{18.11}$$

or

$$\frac{d^2u}{dr^2} = -k^2 u \tag{18.12}$$

which means

$$u(r) = Ae^{ikr} + Be^{-ikr} \quad \text{with} \quad A + B = 1 \text{ (by Eq. 18.10)} \tag{18.13}$$

At this point, we will impose the physical condition that the response of the wave function to the potential is an outgoing spherical wave. Then, we get

$$u(r) = e^{ikr} \tag{18.14}$$

which finally means that

$$G(\vec{r}) = -\frac{e^{ikr}}{4\pi r} \tag{18.15}$$

Note that in this Green's function problem that we just solved, the boundary condition $u(r \to 0) = 0$ (Eq. 17.15) does *not* apply, since we are considering a potential that is as singular as a delta function. Indeed, we *had to* choose $u(r \to 0) = 1$ in the current case, due to the very singular nature of the potential.

Having obtained the Green's function, the full solution for a particular solution is obtained as the convolution of $2mV\psi/\hbar^2$ and G

$$\psi(\vec{r}) = -\frac{m}{2\pi\hbar^2}\int d^3\vec{r}\,'\,\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}V(\vec{r}\,')\,\psi(\vec{r}\,') \qquad \text{a particular solution} \tag{18.16}$$

By adding the homogeneous solution, ψ_h (free particle solution), we get the general solution.

$$\psi(\vec{r}) = \psi_h(\vec{r}) - \frac{m}{2\pi\hbar^2}\int d^3\vec{r}\,'\,\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}V(\vec{r}\,')\,\psi(\vec{r}\,') \qquad \text{general solution} \tag{18.17}$$

Note that, this is the **integral equation form of the Schrödinger equation**. In some sense, we have not done much so far. We just turned the differential equation into the integral equation!

For the scattering problem, the choice for the homogeneous solution is Ae^{ikz}, as in Eq. 16.9.

$$\psi(\vec{r}) = Ae^{ikz} - \frac{m}{2\pi\hbar^2}\int d^3\vec{r}\,'\,\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}V(\vec{r}\,')\,\psi(\vec{r}\,') \quad \text{solution for scattering problem} \tag{18.18}$$

Here, the second part, i.e., the particular solution part, corresponds to $Af(\theta)e^{ikr}/r$ of Eq. 16.9, for large r. We shall investigate this term in more depth now.

18.2 Born approximation

The above solution, Eq. 18.18, is a general solution for the scattering problem[2].

The idea of the Born approximation is a simple perturbation idea. Assuming that V can be taken as a perturbation, we see that Eq. 18.18 can be viewed as a perturbation equation, with $L \equiv \psi - Ae^{ikz}$ and $R \equiv -\frac{m}{2\pi\hbar^2}\int d^3\vec{r}\,'\,\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}V(\vec{r}\,')\,\psi(\vec{r}\,')$, where L and R refer to the two parts of the perturbation equation $L = R$ in page 4 of LN 3.

The perturbation series that can be generated from this equation is called the "Born series" and it again has the intuitive interpretation in terms of Feynman diagram type of picture (page T418 of the textbook).

Here, we will content ourselves with the first order approximation. We can plug in the zeroth order solution $\psi(\vec{r}) \approx Ae^{ikz} \equiv Ae^{i\vec{k}_i\cdot\vec{r}}$ into the integral

$$\psi(\vec{r}) = A\left(e^{ikz} - \frac{m}{2\pi\hbar^2}\int d^3\vec{r}\,'\,\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}V(\vec{r}\,')\,e^{i\vec{k}_i\cdot\vec{r}\,'}\right) \tag{18.19}$$

This is the **first Born approximation**. Note that this equation is valid for any $\vec{r}$. If this first order solution is all we want, then we can now take the asymptotic limit (see the next section). If not, then we must plug this equation into Eq. 18.18 to get the second order correction, and so on and so forth. Note that once one makes the asymptotic limit (large r), then the solution is no longer valid for use in the

[2]Also, the more fundamental equation, Eq. 18.17 can be taken as a bound state solution as well, if the substitution $k \to i\kappa$ is made for $E < 0$ ($\kappa = \sqrt{-2mE}/\hbar$).

perturbation equation, since for the perturbation loop we need to know the previous order solution for all $\vec{r}$ values.

As we already said above, here, we are content with the first order approximation, and so we can take the large r limit (see the next section), and as a result, we get (by using Eq. 18.26)[3]

$$f(\theta,\phi) \approx -\frac{m}{2\pi\hbar^2}\int d^3\vec{r}\,'\, e^{-i(\vec{k}_f-\vec{k}_i)\cdot\vec{r}\,'}\, V(\vec{r}\,') \tag{18.20}$$

which is the Born-approximation formula for scattering amplitude. It is important to note that this approximation is valid as long as V is small. Note that the hard sphere problem that we discussed in the last two lectures can not be treated by Born approximation, since in that case the potential is infinite! For low energy scattering, we can replace the phase factor with 1

$$f(\theta,\phi) \approx -\frac{m}{2\pi\hbar^2}\int d^3\vec{r}\,'\, V(\vec{r}\,') \qquad \text{long wave length} \tag{18.21}$$

If the potential is central, then we get, after effecting the angular integrals by choosing the direction of $\vec{q}$ (defined below) as the z direction,

$$f(\theta) \approx -\frac{2m}{\hbar^2 q}\int_0^\infty dr\, rV(r)\sin(qr) \tag{18.22}$$

with

$$\vec{q} \equiv \vec{k}_f - \vec{k}_i, \quad q \equiv |\vec{q}| = 2k\sin(\theta/2) \tag{18.23}$$

is the change of the wave vector due to scattering.

Note that the scattering amplitude (Eq. 18.20) can be written as

$$f = -\frac{4\pi^2 m}{\hbar^2}\left\langle \vec{k}_f \left|\hat{V}\right| \vec{k}_i\right\rangle \tag{18.24}$$

where $\left|\vec{k}\right\rangle$ is a plane wave state (Dirac-delta-function normalized).

18.3 Asymptotic form

Let us assume that $r \gg$ the range of the potential as we have been assuming so far (page 4, LN 16). It means that we assume $r \gg r'$. We get

$$|\vec{r}-\vec{r}\,'|^2 \approx r^2\left(1 - 2\,\frac{\vec{r}\cdot\vec{r}\,'}{r^2}\right)$$

[3]Note that here, we are entertaining the possibility that the problem regards an open system, with angle dependence on $V(\vec{r}\,')$ and the subsequent ϕ dependence on f.

we get

$$|\vec{r}-\vec{r}\,'| \;\approx\; r\left(1-\frac{\vec{r}\cdot\vec{r}\,'}{r^2}\right)$$

So,

$$e^{ik|\vec{r}-\vec{r}\,'|} \;\approx\; e^{ikr}\, e^{-i\vec{k}_f\cdot\vec{r}\,'} \qquad\qquad \vec{k}_f = \text{the wave vector in the final state} = k\vec{e}_r$$

It is important to note that while, $kr \gg |\vec{k}_f\cdot\vec{r}\,'|$, the second term cannot be ignored in the exponent. The reason is that often $1/k$ is on the order of atomic dimensions, and the factor $e^{-i\vec{k}_f\cdot\vec{r}\,'}$ scans over different positions of the atomic potential, causing *interference* for beams bouncing off at different positions of the potential. All the while, the first exponential factor e^{ikr} is a fixed number if the detector position ($\vec{r}$) is fixed. So, both terms must be kept, since none of the terms can be thought of as ≈ 1 in general [4]. On the other hand, the following is a good approximation

$$\frac{1}{|\vec{r}-\vec{r}\,'|} \;\approx\; \frac{1}{r}$$

Therefore, for $r \gg$ the range of the potential, we see that Eq. 18.18 becomes

$$\psi(\vec{r}) \;=\; Ae^{ikz} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3\vec{r}\,'\, e^{-i\vec{k}_f\cdot\vec{r}\,'}\, V(\vec{r}\,')\,\psi(\vec{r}\,') \tag{18.25}$$

Comparing this with Eq. 16.9, we find that

$$f(\theta,\phi) \;=\; -\frac{m}{2\pi\hbar^2 A}\int d^3\vec{r}\,'\, e^{-i\vec{k}_f\cdot\vec{r}\,'}\, V(\vec{r}\,')\,\psi(\vec{r}\,') \tag{18.26}$$

where we have, for now, left the possibility that $V(\vec{r}\,')$ is angle-dependent, so f is ϕ-dependent as well as θ-dependent, while for a closed system, $V(\vec{r}\,') = V(r')$ from the isotropy of space, and f can depend only on θ (page 3 of LN 16).

While the last equation gives a *formal solution* for $f(\theta,\phi)$, it is *not* a good form for working out perturbation expansion. The reason is that this asymptotic form is valid only for large r, while for the perturbation expansion we need to know ψ *everywhere*. This is why Eq. 18.18 is the fundamental equation to use for the perturbation expansion.

Eq. 18.26 can, and must, be used when you want to finally get the scattering amplitude in the n-th order approximation, when you know the solution ψ fully in the $(n-1)$-th order approximation.

[4] Of course, in the long wave length limit, one can take $e^{-i\vec{k}_f\cdot\vec{r}\,'} \approx 1$.

18.4 Examples

Please follow Examples T11.4–11.6 of the book.