Quantum Many Body Theory

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Week 2

2 Scattering Theory with Green's Functions

2.1 Relation between the scattering amplitude and the T-matrix

Consider a particle moving in a potential $V(x)$ in three dimensions, thus the Hamiltonian is

$$\hat{H} = -\frac{1}{2m}\Delta + V(x),\ \hat{H}\psi = E\psi. \tag{2.1}$$

In quantum mechanics it is shown that the wave function of this particle can have the following asymptotic (at large distance r) behavior:

$$\psi \sim e^{ipz} + \frac{f(\theta)}{r}e^{ipr}. \tag{2.2}$$

Here $p^2/(2m) = E$, z is one of the coordinates of the 3D space, along which an incoming wave e^{ipz} is propagating, $f(\theta)$ is the scattering amplitude, which depends only on the angle θ between $\vec{r}$ and z, but not on the magnitude of $\vec{r}$, denoted as r.

The problem: how does one find $f(\theta)$ given the Green's function $\hat{G}^R$? This is done in the following way. One way to look for a solution of (2.1) is by creating, initially, the incoming wave $e^{ipz} \equiv e^{i\vec{p}\vec{r}}$. Here $\vec{p}$ is a vector directed along the z-coordinate. The incoming wavefunction is not an eigenfunction of the Hamiltonian. Then we let it evolve in time according to the time dependent Schrodinger equation. Eventually it stops depending on time, except for the usual factor e^{-iEt}, and develops the asymptotics (2.2) describing the incoming and the outgoing wave.

Denote $\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{H}_0 = -\frac{1}{2m}\Delta$. G_0^R will denote the retarded Green's function of H_0, while G^R is reserved for the full Green's function.

By the definition of the time-dependent retarded Green's function,

$$\psi(t,\vec{r}) = i\int d^3r'\ G^R(\vec{r},\vec{r}',t)e^{i\vec{p}\vec{r}'} = i\int \frac{d^3r'dE}{2\pi}\ G^R(\vec{r},\vec{r}',E)e^{i\vec{p}\vec{r}'-iEt} \tag{2.3}$$

In the Fourier space, the initial wave function $\psi_0(\vec{r}) = e^{i\vec{p}\vec{r}}$ is nothing but $\psi_0(\vec{k}) = \delta(\vec{k}-\vec{p})$. We go into Fourier space, and recall that the Fourier transform of the noninteracting Green's function is given by

$$\left\langle \vec{k}\right| \hat{G}_0^R \left|\vec{k}'\right\rangle = \frac{2\pi\delta(\vec{k}-\vec{k}')}{E + i0 - \frac{k^2}{2m}}. \tag{2.4}$$

However, for brevity, this delta-function is often omitted and the following notation is introduced

$$G_0^R(k,E) = \frac{1}{E + i0 - \frac{k^2}{2m}}. \tag{2.5}$$

Now recall the definition of the T-matrix, $\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{T} \hat{G}_0$. With its help this becomes

$$\psi(\vec{r}, t) = i \int \frac{dE}{2\pi}\ G_0^R(p, E) e^{i\vec{p}\vec{r} - iEt} + i \int \frac{d^3k dE}{(2\pi)^4} G_0^R(k, E) T(\vec{k}, \vec{p}, E) G_0^R(p, E) e^{i\vec{k}\vec{r} - iEt}. \quad (2.6)$$

This is the solution to the problem of representing the scattering problem in terms of Green's functions. We can also write it in a different way by denoting the Fourier time transform of the wave function by

$$\psi(\vec{r}, E) = i G_0^R(p, E) e^{i\vec{p}\vec{r}} + i \int \frac{d^3k}{(2\pi)^3} G_0^R(k, E) T(\vec{k}, \vec{p}, E) G_0(p, E) e^{i\vec{k}\vec{r}}. \quad (2.7)$$

The first term in this expression is trivial: it represents the initial wave propagating in time. And indeed, recalling that $G_0^R = 1/(E - p^2/(2m) + i0)$, we can take the integral in the first term of (2.6) over E by residues to get

$$e^{i\vec{p}\vec{r} - i\frac{p^2}{2m}t}. \quad (2.8)$$

The second term represents the scattered wave. To evaluate it we need to know the T-matrix, which depends in some unknown way on the potential V. So it would appear that until we figure out T for a specific problem, no further progress is possible. This is true, however if all we are interested in is a large r asymptotics of the wave function in the far future, this can be simplified further.

The integral over $\vec{k}$ consists of angular integration and integration over the magnitude of k. The angular integration involves the term $e^{i\vec{k}\vec{r}} = e^{ikr\cos(\theta)}$, where θ is the angle of $\vec{k}$ counted from the direction of $\vec{p}$, direction of the incoming wave. The integral itself goes over $\sin(\theta) d\theta$. $T(\vec{k}, \vec{p}, E)$ also depends on θ in some unknown way, making taking this integral impossible. However, $e^{ikr\cos(\theta)}$ is a fast oscillating function of θ, if r is large. We will thus employ the steepest descend method which says that only a vicinity of the point where the first derivative of $\cos(\theta)$ vanishes which is important. There are two such points, $\theta = 0$ and $\theta = \pi$. Take the first such point. There we write

$$\int \sin(\theta) e^{ikr\cos(\theta)} \approx \int_0^\infty \theta d\theta\ e^{ikr\left(1 - \theta^2/2\right)} = \frac{e^{ikr}}{ikr} \quad (2.9)$$

Similarly, the second point gives

$$\int \sin(\theta) e^{-ikr\cos(\theta)} \approx \int_0^\infty \theta d\theta\ e^{-ikr\left(1 - \theta^2/2\right)} = -\frac{e^{-ikr}}{ikr} \quad (2.10)$$

Thus we find, as far as the second term in (2.7) is concerned

$$i\int_0^\infty \frac{k^2 dk}{4\pi^2}\frac{e^{ikr}T(k,p,\theta=0,E)-e^{-ikr}T(k,p,\theta=\pi,E)}{ikr}\frac{1}{E+i0-k^2/(2m)}\frac{1}{E+i0-p^2/(2m)}. \tag{2.11}$$

We observe that the second term can be interpreted as the integral over negative k. Combining the terms together thus gives

$$i\int_{-\infty}^\infty \frac{kdk}{4\pi^2}\frac{e^{ikr}T(k,p,E)}{ir}\frac{1}{E+i0-k^2/(2m)}\frac{1}{E+i0-p^2/(2m)}. \tag{2.12}$$

Next step is to do the integral over k. We do it by residues: closing the k-contour over the upper half plane, the only pole which contributes is $k=\sqrt{2mE}+i0$. This gives

$$-i\frac{m}{2\pi r}T(k,p,E)\frac{e^{ir\sqrt{2mE}}}{E+i0-p^2/(2m)}. \tag{2.13}$$

Finally this gives for the wave function

$$-i\frac{m}{2\pi}\int \frac{dE}{2\pi r}T(k,p,E)\frac{e^{ir\sqrt{2mE}}}{E+i0-p^2/(2m)}e^{-iEt}=-\frac{m}{2\pi r}T(k,p,E=p^2/(2m))e^{-i\frac{p^2}{2m}t}e^{irp} \tag{2.14}$$

To do the integral over E, we assumed that the only pole in the lower half plane is $E=p^2/(2m)-i0$. This is in fact not completely true: there could be poles of $T(k,p,E)$ in the lower half plane. However, those will give contributions at energy which is not $p^2/(2m)$ which we will ignore because we would like to study scattering at $E=p^2/(2m)$.

We emphasize that the T-matrix which sits in this expression must be evaluated with an incoming momentum $\vec{p}$, and the outgoing momentum $\vec{k}$, whose length is p, and whose direction parallels $\vec{r}$. Comparison with (2.2) gives, finally,

$$f(\theta)=-\frac{m}{2\pi}T(\theta). \tag{2.15}$$

This is the relation we need, which connects the T-matrix to the scattering amplitude. Here θ is the angle between the direction of the incoming wave and the direction of $\vec{r}$, just as in (2.2).

2.2 Scattering in a delta-function potential in 3D

Let us solve the problem of scattering in 3D in a delta function potential

$$\hat{H}=-\frac{1}{2m}\Delta+\lambda\delta(\vec{r}). \tag{2.16}$$

We need to compute the T-matrix. The calculation proceeds completely equivalent to the calculation of T-matrix in the 1D case, which was studied in Week 1 notes. The only difference is in the integral

$$\Pi = \int \frac{d^3k}{(2\pi)^3} \frac{1}{E - \frac{k^2}{2m} + i0}, \tag{2.17}$$

which now must be done in 3D, not in 1D.

This integral is divergent and does not make sense. This reflects the following well known fact: the delta-function potential in 3D is not a well defined potential. However, let us imagine that this potential is similar to a delta-function, but has a finite extend in space. Then its Fourier transform will be λ at low momenta, and quickly go to zero when momenta exceed Λ, where Λ is the inverse extend of the potential. Then the integral becomes

$$\Pi = \int_0^\Lambda \frac{k^2 dk}{2\pi^2} \frac{1}{E - \frac{k^2}{2m} + i0} = \int_0^\Lambda \frac{dk}{2\pi^2} \frac{k^2 - 2mE}{E - \frac{k^2}{2m} + i0} + \int_0^\Lambda \frac{dk}{2\pi^2} \frac{2mE}{E - \frac{k^2}{2m} + i0}. \tag{2.18}$$

This gives

$$\Pi = -\frac{m\Lambda}{\pi^2} + 2mE \int_0^\Lambda \frac{dk}{2\pi^2} \frac{1}{E - \frac{k^2}{2m} + i0}. \tag{2.19}$$

The integral is convergent and can be extended to infinity as long as $E \ll \Lambda^2/(2p)$. It can also be extended to minus infinity, at the expense of introducing an extra factor of 2. With the help of (1.39) of Week 1, we now find

$$\Pi = -\frac{m\Lambda}{\pi^2} - \frac{2mE}{2\pi} \sqrt{\frac{m}{-2E}}. \tag{2.20}$$

The expression (1.40) of Week 1 gives

$$T = \frac{1}{\frac{1}{\lambda} + \frac{m\Lambda}{\pi^2} + \frac{mE}{\pi}\sqrt{\frac{m}{-2E}}}. \tag{2.21}$$

Notice that it is completely independent of the angle θ, and depends only on the scattering energy E. Substituting $E = p^2/(2m)$ gives

$$f = -\frac{m}{2\pi} T = \frac{1}{-\frac{2\pi}{m\lambda} - \frac{2\Lambda}{\pi} - ip}. \tag{2.22}$$

Thus the scattering is angle independent (fully s-wave) and proceeds with the scattering length

$$a = \left(\frac{2\pi}{m\lambda} + \frac{2\Lambda}{\pi} \right)^{-1}. \tag{2.23}$$

Indeed, the scattering length is defined as $a = -f(p = 0)$.

The poles of the T matrix reflect the bound states, as usual. Examining (2.21) we find that the poles are possible only if

$$\lambda < -\frac{\pi^2}{m\Lambda}. \tag{2.24}$$

That is, the delta function must be strong enough and attractive for the bound state to appear. When $\lambda = -\pi^2/(m\Lambda)$, the scattering length is equal to infinity and the scattering amplitude is equal to

$$f = -\frac{1}{ip}. \tag{2.25}$$

This is called the unitary limit of scattering.