Scattering in quantum mechanics

1 The Lippmann-Schwinger equation

We are interested in a theory that can describe the scattering of a particle from a potential $V(\mathbf{x})$. Our Hamiltonian is

$$H = H_0 + V.$$

where H_0 is the free-particle kinetic energy operator

$$H_0 = \frac{p^2}{2m}.$$

In the absence of V the solutions of the Hamiltonian could be written as the free-particle states satisfying $H_0|\phi\rangle = E|\phi\rangle$. These free-particle eigenstates could be written as momentum eigenstates $|\mathrm{p}\rangle$, but since that isn't the only possibility we hold off writing an explicit form for $|\phi\rangle$ for now. The full Schrödinger equation is

$$H_0 + V|\phi\rangle = E|\phi\rangle.$$

We define these eigenstates of H such that $|\psi\rangle \rightarrow |\phi\rangle$ as $V \rightarrow 0$, where $|\phi\rangle$ and $|\psi\rangle$ have the same energy eigenvalue. (We are able to do this since the spectra of both H and $H+V$ are continuous.)

A possible solution is[1]

$$|\psi\rangle = \frac{1}{E - H_0} V|\psi\rangle + |\phi\rangle. \tag{1}$$

By multiplying by $(E - H_0)$ we can show that this looks fine, other than the problem of the operator $1/(E - H_0)$ being singular. The singular behaviour in (1) can be fixed by making E slightly complex and defining

$$\boxed{|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{(\pm)}\rangle}. \tag{2}$$

This is the **Lippmann-Schwinger** equation. We will find the physical meeting of the $(\pm)$ in the $|\psi^{(\pm)}\rangle$ shortly.

2 Scattering amplitudes

To calculate scattering amplitudes we are going to have to use both the position and the momentum basis, because $|\phi\rangle$ is a momentum eigenstate, and V is a function

[1] Remember that functions of operators are defined by $f(\hat{A}) = \sum_i f(a_i)|a_i\rangle\langle a_i|$.

of $\mathbf{x}$. If $|\phi\rangle$ stands for a plane wave with momentum $\hbar\mathbf{k}$ then the wavefunction can be written

$$\langle \mathbf{x}|\phi\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{\frac{3}{2}}}.$$

We can express (2) in the position basis by bra-ing through with $\langle \mathbf{x}|$ and inserting the identity operator $\int d^3x'\,|\mathbf{x}'\rangle\langle\mathbf{x}'|$

$$\langle \mathbf{x}|\psi^{(\pm)}\rangle = \langle \mathbf{x}|\phi\rangle + \int d^3x' \left\langle \mathbf{x}\right|\frac{1}{E - H_0 \pm i\epsilon}\left|\mathbf{x}'\right\rangle \langle \mathbf{x}'|V|\psi^{(\pm)}\rangle. \tag{3}$$

In the problem set we will show that the solution to the Green's function defined by

$$G_{\pm}(\mathbf{x},\mathbf{x}') \equiv \frac{\hbar^2}{2m}\left\langle \mathbf{x}\right|\frac{1}{E - H_0 \pm i\epsilon}\left|\mathbf{x}'\right\rangle$$

is given by

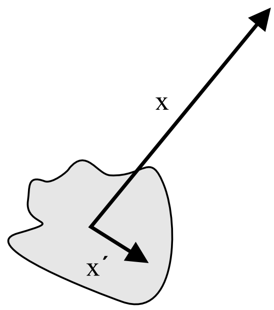
$$G_{\pm}(\mathbf{x},\mathbf{x}') = -\frac{1}{4\pi}\frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}.$$

Using this result we can see that the amplitude of interest simplifies to

$$\langle \mathbf{x}|\psi^{(\pm)}\rangle = \langle \mathbf{x}|\phi\rangle - \frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3x' \frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} V(\mathbf{x}')\langle \mathbf{x}'|\psi^{(\pm)}\rangle \tag{4}$$

where we have also assumed that the potential is *local* in the sense that it can be written as

$$\langle \mathbf{x}'|V|\mathbf{x}''\rangle = V(\mathbf{x}')\delta^3(\mathbf{x}'-\mathbf{x}'').$$



The wave function (4) is a sum of two terms. The first is the incoming plane wave. For large $|\mathbf{x}|$ the spatial dependence of the second term is $e^{\pm ikr}/r$. We can now understand the physical meaning of the $|\psi^{(\pm)}\rangle$ states; they represent outgoing $(+)$ and incoming $(-)$ spherical waves respectively. We are interested in the *outgoing* $(+)$ spherical waves – the ones which have been scattered from the potential.

We want to know the amplitude of the outgoing wave at a point $\mathbf{x}$. For pratical experiments the detector must far from the scattering centre in the sense so we can assume $|\mathbf{x}| \gg |\mathbf{x}'|$.

We define a unit vector in the direction of the observation point

$$\hat{\mathbf{r}} = \frac{\mathbf{x}}{|\mathbf{x}|}$$

and also a wave-vector for particles travelling in the direction $\hat{\mathbf{x}}$,

$$\mathbf{k}' = k\hat{\mathbf{r}}.$$

Far from the scattering centre we can write

$$\begin{aligned} |\mathbf{x}-\mathbf{x}'| &= \sqrt{r^2 - 2rr'\cos\alpha + r'^2} \\ &= r\sqrt{1 - 2\frac{r'}{r}\cos\alpha + \frac{r'^2}{r^2}} \\ &\approx r - \hat{\mathbf{r}}\cdot\mathbf{x}' \end{aligned}$$

where α is the angle between the $\mathbf{x}$ and the $\mathbf{x}'$ directions.

It's safe to replace the $|\mathbf{x} - \mathbf{x}|$ in the denominator in the integrand of (4) with just r, but the phase term will need to be replaced by $r - \hat{\mathbf{r}} \cdot \mathbf{x}'$. So we finally simplify the wave function to

$$\langle \mathbf{x}|\psi^{(+)}\rangle \xrightarrow{r \text{ large}} \langle \mathbf{x}|\mathbf{k}\rangle - \frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{e^{ikr}}{r}\int d^3x'\, e^{i\mathbf{k}'\cdot\mathbf{x}'}V(\mathbf{x}')\langle \mathbf{x}'|\psi^{(+)}\rangle$$

which we can write as

$$\langle \mathbf{x}|\psi^{(+)}\rangle = \langle \mathbf{x}|\psi^{(+)}\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}}\left[e^{i\mathbf{k}\cdot\mathbf{x}} + \frac{e^{ikr}}{r}f(\mathbf{k},\mathbf{k}')\right].$$

This makes it clear that we have a sum of an incoming plane wave and an outgoing spherical wave with amplitude $f(\mathbf{k}',\mathbf{k})$ given by

$$f(\mathbf{k}',\mathbf{k}) = -\frac{1}{4\pi}(2\pi)^3\frac{2m}{\hbar^2}\langle \mathbf{k}|V|\psi^{(\pm)}\rangle. \tag{5}$$

$\langle \mathbf{x}|\phi\rangle \propto e^{ik|\mathbf{x}|}/|\mathbf{x}|$

Wave function of an outgoing spherical wave.

We will ignore the interference between the first term which represents the original 'plane' wave and the second term which represents the outgoing 'scattered' wave. From (4) the scattered wave has an amplitude $f(\mathbf{k}',\mathbf{k})$ given by So we find that the partial cross-section $d\sigma$ – the number of particles scattered into a particular region of solid angle per unit time divided by the incident flux[2] – is given by

$$d\sigma = \frac{r^2|j_{\text{scatt}}|}{|j_{\text{incid}}|}d\Omega = |f(\mathbf{k}',\mathbf{k})|^2\, d\Omega.$$

3 The Born approximation

If the potential is weak we can assume that the eigenstates are only slightly modified by V, and so we can replace $|\psi^{(\pm)}\rangle$ in (5) by $|\mathbf{k}\rangle'$.

$$f^{(1)}(\mathbf{k}',\mathbf{k}) = -\frac{1}{4\pi}(2\pi)^3\frac{2m}{\hbar^2}\langle \mathbf{k}|V|\mathbf{k}'\rangle. \tag{6}$$

This is known as the **Born approximation**. Within this approximation we have found the nice simple result

$$\boxed{f^{(1)}(\mathbf{k}',\mathbf{k}) \propto \langle \mathbf{k}|V|\mathbf{k}'\rangle}.$$

Up to some constant factors, the scattering amplitude is found by squeezing the perturbing potential V between incoming and the outgoing momentum eigenstates of the free-particle Hamiltonian.

[2]Remember that the flux is given by $\mathbf{j} = \frac{\hbar}{2im}[\psi^*\nabla\psi - \psi\nabla\psi^*]$.

Expanding out (6) in the position representation (by insertion of a couple of completeness relations $\int d^3x' \, |\mathbf{x}'\rangle\langle\mathbf{x}'|$) we can write

$$f^{(1)}(\mathbf{k}',\mathbf{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3x' e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}'}V(\mathbf{x}').$$

This result is telling us that scattering amplitude is proportional to the 3d *Fourier transform* of the potential.

4 Beyond Born: propagators

To see how things develop if we don't want to rashly assume that $|\psi^{\pm}\rangle \approx |\phi\rangle$ it is useful to define a **transition operator** T such that

$$V|\psi^{(+)}\rangle = T|\phi\rangle$$

Multiplying the Lippmann-Schwinger equation (2) by V we get an expression for T

$$T|\phi\rangle = V|\phi\rangle + V\frac{1}{E - H_0 + i\epsilon}T|\phi\rangle.$$

Since this is to be true for any $|\phi\rangle$, the corresponding operator equation must also be true:

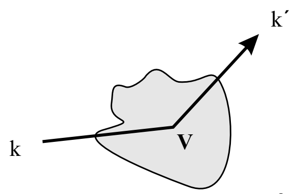
$$T = V + V\frac{1}{E - H_0 + i\epsilon}T.$$

This operator is defined recursively. It is is exactly what we need to find the scattering amplitude, since from (5), the amplitude is given by

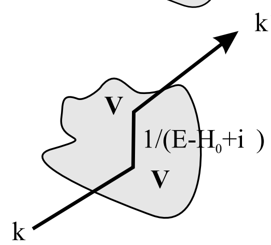
$$f(\mathbf{k}',\mathbf{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\langle\mathbf{k}'|T|\mathbf{k}\rangle.$$

We can now find an iterative solution for T:

$$T = V + V\frac{1}{E - H_0 + i\epsilon}V + V\frac{1}{E - H_0 + i\epsilon}V\frac{1}{E - H_0 + i\epsilon}V + \dots \qquad (7)$$



We can interpret this series of terms as a sequence of the operators corresponding to the particle interacting with the potential (operated on by V) and propagating along for some distance (evolves according to $\frac{1}{E-H_0+i\epsilon}$).



The operator

$$\boxed{\frac{1}{E - H_0 + i\epsilon}} \qquad (8)$$

is known as the **propagator**. Propagators are central to much of what we will do later on, so it is a good idea to try to work out what they mean. Physically the propagator can be thought of as a term in the expansion (7) which is giving a contribution the amplitude for a particile moving from an interaction at point A to another at point B. Mathematically it is a Green's function solution to the Lippmann-Schwinger in the position representation (3).

We are now in a position to quantify what we meant by a 'weak' potential earlier on. From the expansion (7) we can see that the first Born approximation (6) will be useful if the matrix elements of T can be well approximated by its first term V.

When is this condition likely to hold? Remember that the Yukawa potential was proportional to the square of a dimensionless coupling constant $\propto g^2$. If $g^2 \ll 1$ then successive applications of V introducing higher and higher powers of g and can usually be neglected. This will be true for electromagnetism, since the dimensionless coupling relevant for electromagnetism is related to the fine structure constant

$$\frac{g^2}{4\pi} = \alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137}.$$

Since $\alpha \approx\ll 1$, we can usually get away with just the first term of (7) for electric interactions (i.e. we can use the Born approximation).

5 Strong potentials

The strong nuclear force has a coupling constant $\alpha_s \sim 1$. In such cases the terms in T with multiple powers of V are likely to be of approximately the same size as the leading Born term, and the expansion (7) is not a sensible way to proceed.

Nevetheless it is still possible to make progress by making use of rotational invariance and conservation of probability. By expressing the incoming wave as a sum of spherical harmonics with different orbital momentum quantum numbers l, the maximum partial cross-section for each harmonic is found to be (see e.g. Section 7.6 of Sakurai)

$$\sigma^{(l)}_{\max} = 4\pi \left(\frac{\lambda}{2\pi}\right)^2 (2l+1).$$

Key concepts

- The amplitude for scattering from a potential can be solved iteratively, using the **Lippman-Schwinger** equation:

$$\boxed{|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\epsilon} V |\psi^{(\pm)}\rangle}$$

- Collisions can be characterised as a sum over one or more point interactions (governed by V) interspersed with free-particle propagation described by a **propagator**

$$\boxed{\frac{1}{E - H_0 + i\epsilon}}$$

- If the interaction is sufficiently weak (i.e. has a **coupling constant** $\ll 1$) we can approximate the scattering amplitude by the first term (V) or terms in an operator expansion.

- The scattering amplitude between the 'free-particle' eigenstates $|\mathbf{k}\rangle \to |\mathbf{k}'\rangle$ is given in the leading **Born approximation** by

$$\boxed{f^{(1)}(\mathbf{k}', \mathbf{k}) \propto \langle \mathbf{k}'|V|\mathbf{k}\rangle}$$

which is the **Fourier transform** of the potential.

- The differential cross-section is given in terms of the scattering amplitude by

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\mathbf{k}', \mathbf{k})|^2}$$

References

- J.J. Sakurai. "Modern quantum mechanics". Chapter 7 forms the basis for this handout.
- M.G. Bowler, "Femtophysics". Opens with a less mathematical description of this method.
- Binney and Skinner, "The physics of quantum mechanics", Chapter 12. The $\pm i\epsilon$ perscription can be better understood using the S-matrix formalism explained in Chapter 12.
- Lippmann and Schwinger, Phys.Rev.79:469-480,1950. The masochistic may be interested to see the original derivation of (2) using a path-integral technique.