NOTES ON 1-PARTICLE SCATTERING

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1. The resolvent and the propagator

Given a Hamiltonian $\hat{H}$, the resolvent and time-propagator are the operators:

$$\hat{g}(z) = (z - \hat{H})^{-1} \quad z \notin \sigma(H) \tag{1}$$

$$\hat{U}(t) = \exp(-\tfrac{i}{\hbar} t\hat{H}) \quad t \in \mathbb{R} \tag{2}$$

The matrix element $g(\mathbf{x}, \mathbf{x}'; z) = \langle \mathbf{x}|\hat{g}(z)|\mathbf{x}'\rangle$ is a Green function. For a local Hamiltonian it solves:

$$(z - H_{\mathbf{x}})g(\mathbf{x}, \mathbf{x}'; z) = \delta(\mathbf{x} - \mathbf{x}') \tag{3}$$

and has spectral representation

$$g(\mathbf{x}, \mathbf{x}'; z) = \sum_a \frac{\langle \mathbf{x}|a\rangle\langle a|\mathbf{x}'\rangle}{z - E_a} + \int_{\sigma_c} dE' \, \frac{A(\mathbf{x}, \mathbf{x}'; E')}{z - E'}$$

For real z the poles and cuts are avoided by adding them infinitesimal imaginary parts. This can be done in different ways that define different Green functions. Their difference is a solution of the homogeneous equation $(z - H_{\mathbf{x}})\Delta g(\mathbf{x}, \mathbf{x}'; z) = 0$.

In the retarded resolvent $\hat{g}^R(E) = \hat{g}(E + i\eta)$ all singularities are shifted to the lower half-plane. The retarded Green function is analytic in the upper half plane. It is the Fourier transform of an amplitude for the propagation forward in time:

$$\int_{\mathbb{R}} \frac{dE}{2\pi i} g^R(\mathbf{x}, \mathbf{x}'; E)e^{-\frac{i}{\hbar}Et} = -\theta(t)\langle \mathbf{x}|\hat{U}(t)|\mathbf{x}'\rangle \tag{4}$$

The advanced resolvent is $\hat{g}^A(E) = \hat{g}(E - i\eta) = \hat{g}^R(E)^\dagger$. The advanced Green function $g^A(\mathbf{x}, \mathbf{x}'; E)$ is analytic in the lower half-plane, and it is the Fourier transform of the amplitude for the propagation backward in time.

For $\hat{H}_0 = \hat{p}^2/2m$, the retarded Green function is

$$\boxed{g_0^R(\mathbf{x}, \mathbf{x}'; E) = \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}}{E - E(\mathbf{k}) + i\eta} = -\frac{m}{2\pi\hbar^2} \frac{\exp(ik_E|\mathbf{x} - \mathbf{x}'|)}{|\mathbf{x} - \mathbf{x}'|}} \tag{5}$$

where $k_E = \sqrt{2mE}/\hbar$.

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2. The T matrix

Consider the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$, and the resolvent operators $\hat{g}(z)$ and $\hat{g}_0(z)$. From $1 = (z - \hat{H}_0 - \hat{V})\hat{g}(z)$ the following identity is obtained:

$$\boxed{\hat{g}(z) = \hat{g}_0(z) + \hat{g}_0(z)\hat{V}\hat{g}(z)} \tag{6}$$

It is also $\hat{g}(z) = \hat{g}_0(z) + \hat{g}(z)\hat{V}\hat{g}_0(z)$. The formal solution by iteration (Born expansion), being convergent or not, introduces the operator $\hat{T}(z)$ (a total self-energy):

$$\begin{aligned}
\hat{g}(z) =& \hat{g}_0 + \hat{g}_0(\hat{V} + \hat{V}\hat{g}_0\hat{V} + \hat{V}\hat{g}_0\hat{V}\hat{g}_0\hat{V} + ...)\hat{g}_0 \\
=& \hat{g}_0 + \hat{g}_0\hat{T}(z)\hat{g}_0 \\
\hat{T}(z) =& \hat{V} + \hat{V}\hat{g}_0(z)\hat{V} + \hat{V}\hat{g}_0(z)\hat{V}\hat{g}_0(z)\hat{V} + ...
\end{aligned}$$

Then: $\hat{T}(z)\hat{g}_0(z) = \hat{V}\hat{g}(z)$ and $\hat{T}(z) = \hat{V} + \hat{V}\hat{g}_0(z)\hat{T}(z) = \hat{V} + \hat{T}(z)\hat{g}_0\hat{V}$.

The **T-matrix** is $\hat{T}(E+i\eta)$, which we write as $\hat{T}(E)$. This operator is important in scattering theory. It is

$$\hat{T}(E) = \hat{V} + \hat{V}\hat{g}_0^R(E)\hat{V} + \hat{V}\hat{g}_0^R(E)\hat{V}\hat{g}_0^R(E)\hat{V} + ... \tag{7}$$

We derive an important identity:

Proposition 1.

$$\boxed{\hat{T}(E) - \hat{T}(E)^\dagger = -2\pi i\, \hat{T}(E)^\dagger\, \delta(E - \hat{H}_0)\hat{T}(E)} \tag{8}$$

Proof. The equations for $\hat{T}(E)$ and the adjoint are:

$$\begin{aligned}
\hat{T}(E) &= \hat{V} + \hat{V}\hat{g}_0^R(E)\hat{T}(E) \\
\hat{T}(E)^\dagger &= \hat{V} + \hat{T}(E)^\dagger\hat{g}_0^A(E)\hat{V}
\end{aligned}$$

Right-multiply the second one by $\hat{g}_0^R(E)\hat{T}(E)$ and left-multiply the first one by $\hat{T}(E)^\dagger\hat{g}_0^A(E)$, and subtract:

$$\hat{T}^\dagger(\hat{g}_0^R - \hat{g}_0^A)\hat{T} = \hat{V}\hat{g}_0^R\hat{T} - \hat{T}^\dagger\hat{g}_0^A\hat{V}$$

It is $\hat{V}\hat{g}_0^R\hat{T} = \hat{T} - \hat{V}$ and $\hat{T}^\dagger\hat{g}_0^A\hat{V} = \hat{T}^\dagger - \hat{V}$. Then: $\hat{T}^\dagger(\hat{g}_0^R - \hat{g}_0^A)\hat{T} = \hat{T} - \hat{T}^\dagger$. The difference of the retarded and advanced resolvents is $-2\pi i\, \delta(E - \hat{H}_0)$. □

If $\hat{H}_0 = \hat{p}^2/2m$, the matrix element with momentum eigenstates $\hat{\mathbf{p}}|\mathbf{k}\rangle = \hbar\mathbf{k}|\mathbf{k}\rangle$ is:

$$\begin{aligned}
\langle\mathbf{k}|\hat{T}(E) - \hat{T}(E)^\dagger|\mathbf{k}'\rangle =& -2\pi i \int d\mathbf{q}\langle\mathbf{k}|\hat{T}(E)^\dagger|\mathbf{q}\rangle\, \delta(E - E(q))\langle\mathbf{q}|\hat{T}(E)|\mathbf{k}'\rangle \\
=& -2\pi i\, \frac{mq_E}{\hbar^2}\int d\Omega\, \langle\mathbf{k}|\hat{T}(E)^\dagger|q_E\mathbf{n}\rangle\, \langle q_E\mathbf{n}|\hat{T}(E)|\mathbf{k}'\rangle
\end{aligned} \tag{9}$$

where $d\mathbf{q} = q^2 dq\, d\Omega$ and $q_E = \frac{1}{\hbar}\sqrt{2mE}$. This is a generalized version of the optical theorem, due to W. Heisenberg. In particular, for $\mathbf{k} = \mathbf{k}'$:

$$\mathrm{Im}\,\langle\mathbf{k}|\hat{T}(E)|\mathbf{k}\rangle = -\pi\,\frac{mq_E}{\hbar^2}\int d\Omega\, |\langle q_E\mathbf{n}|\hat{T}(E)|\mathbf{k}\rangle|^2 \tag{10}$$

3. **The scattering problem**

We study the scattering problem for a Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ where $\hat{H}_0 = \hat{p}^2/2m$ and $\hat{V}$ is a short range radial potential. The scattering event is described by a solution $\hat{U}(t)|\psi^+\rangle$ of Schrödinger's equation with the following asymptotic features:
- in the far past it is an in-coming wave packet (far enough to be off the potential range) evolving in time with $\hat{H}_0$,
- in the far future it is the superposition of an undisturbed packet and a scattered wave-function, both far enough to evolve with $\hat{H}_0$,

$$\hat{U}(t)|\psi^+\rangle = \begin{cases} \hat{U}_0(t)|\psi_{\rm in}\rangle & t \to -\infty \\ \hat{U}_0(t)|\psi_{\rm out}\rangle & t \to +\infty \end{cases} \tag{11}$$

with $|\psi_{\rm out}\rangle = |\psi_{\rm in}\rangle + |\psi_{\rm scatt}\rangle$. The statements are made precise through the introduction of the isometries (Möller operators):

$$\hat{\Omega}_\pm = \lim_{t\to\pm\infty} \hat{U}(t)^\dagger \hat{U}_0(t) = \hat{U}_I(\pm\infty, 0)^\dagger \tag{12}$$

where $\hat{U}(t,0) = \hat{U}_0(t,0)\hat{U}_I(t,0)$ defines the interaction propagator.
Then $|\psi^+\rangle = \hat{\Omega}_-|\psi_{\rm in}\rangle$ and $|\psi^+\rangle = \hat{\Omega}_+|\psi_{\rm out}\rangle$. The Möller operators are isometries as they map the full Hilbert space of in/out states of free particles (the asymptotic states) to the continuous subspace of $\hat{H}$, which may also have a subspace spanned by bound states.
The in/out free particle states are connected by the **scattering matrix**:

$$\boxed{|\psi_{\rm out}\rangle = \hat{S}|\psi_{\rm in}\rangle}$$

$$\hat{S} = \hat{\Omega}_+^\dagger \hat{\Omega}_- = \hat{U}_I(\infty, -\infty)$$

Let me only mention here the beautiful RAGE theorem (Ruelle, Amrein, Enns, Georgescu), which characterizes the continuum subspace of $\hat{H}$ as the states ψ for which the time average of the probability of being inside a ball of radius R vanishes:

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T dt \|\hat{P}_R \psi(t)\|^2 = 0$$

$\hat{P}_R$ is the projection of the state in the ball of radius R. It means that the position probability escapes to infinity.

To this description in time it corresponds a description in energy. The solution $\hat{U}(t)|\psi^+\rangle$ is a superposition of stationary states belonging to the continuum spectrum $E > 0$ of $\hat{H}$:

$$\hat{U}(t)|\psi^+\rangle = \int d\mathbf{k}\, c_{\mathbf{k}} \exp(-\tfrac{i}{\hbar}E_k t)|\psi^+_{\mathbf{k}}\rangle \tag{13}$$

$$(E_k - \hat{H}_0)|\psi^+_{\mathbf{k}}\rangle = \hat{V}|\psi^+_{\mathbf{k}}\rangle \tag{14}$$

with coefficients $c_{\mathbf{k}} = \langle \mathbf{k}|\psi_{\rm in}\rangle$ and energy values $E_k = \hbar^2 k^2/2m$.
The eigenvalue equation is formally inverted with the free resolvent, with a contribution of the homogeneous equation $(E_k - \hat{H}_0)|\mathbf{k}\rangle = 0$:

$$|\psi^+_{\mathbf{k}}\rangle = |\mathbf{k}\rangle + \hat{g}^R_0(E_k)\hat{V}|\psi^+_{\mathbf{k}}\rangle \tag{15}$$

In the coordinate representation it is an integral (Lippmann-Schwinger) equation:

$$\psi^+_{\mathbf{k}}(\mathbf{x}) = \langle \mathbf{x}|\mathbf{k}\rangle + \int d\mathbf{x}' g^R_0(\mathbf{x},\mathbf{x}'; E_k) V(\mathbf{x}')\psi^+_{\mathbf{k}}(\mathbf{x}')$$

The choice of the retarded resolvent is intentional: it implies the boundary condition. By eq.(15), the time evolution (13) has two terms:

$$\hat U(t)|\psi^+\rangle = \hat U_0(t)|\psi_{\rm in}\rangle + \int d\mathbf{k}\, c_{\mathbf{k}} \exp(-\tfrac{i}{\hbar}E_k t)\hat g^R_0(E_k)\hat V|\psi^+_{\mathbf{k}}\rangle$$

The second term is the time evolution of a scattered wave-packet that vanishes in the past (see Weinberg, page 205).

We are interested in the far future. For large $r = |\mathbf{x}|$ we expand the Green function g^R for $r \gg |\mathbf{x}'|$, as the potential bounds the integral in $\mathbf{x}'$ in a finite region. With $\mathbf{k}' = k_E\mathbf{n}$, $\mathbf{n} = \mathbf{x}/r$, we obtain:

$$\begin{aligned}
\psi^+_{\mathbf{k}}(\mathbf{x}) &\approx \langle \mathbf{x}|\mathbf{k}\rangle - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d\mathbf{x}' e^{-i\mathbf{k}'\cdot\mathbf{x}'}V(\mathbf{x}')\psi^+_{\mathbf{k}}(\mathbf{x}') \\
&= \langle \mathbf{x}|\mathbf{k}\rangle - \frac{m\sqrt{2\pi}}{\hbar^2}\frac{e^{ikr}}{r}\int d\mathbf{x}'\langle \mathbf{k}'|\mathbf{x}'\rangle\langle \mathbf{x}'|\hat V|\psi^+_{\mathbf{k}}\rangle \\
&= \frac{1}{(2\pi)^{3/2}}\left[e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{4\pi^2 m}{\hbar^2}\frac{e^{ikr}}{r}\langle \mathbf{k}'|\hat V|\psi^+_{\mathbf{k}}\rangle\right] \\
&= \frac{1}{(2\pi)^{3/2}}\left[e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{4\pi^2 m}{\hbar^2}\frac{e^{ikr}}{r}\langle \mathbf{k}'|\hat T(E_k)|\mathbf{k}\rangle\right] \qquad (16)
\end{aligned}$$

The last line descends from (15): $\hat V|\psi^+_{\mathbf{k}}\rangle = \hat V|\mathbf{k}\rangle + \hat V\hat g^R_0(E_k)\hat V|\psi^+_{\mathbf{k}}\rangle$; the equation has formal solution $\hat V|\psi^+_{\mathbf{k}}\rangle = (\hat V + \hat V\hat g^R_0(E_k)\hat V + \ldots)|\mathbf{k}\rangle = \hat T(E_k)|\mathbf{k}\rangle$.

In scattering theory the state $\psi^+_{\mathbf{k}}(\mathbf{x})$ is written as a superposition of a plane wave and a spherical wave weighted by a scattering amplitude that depends on the scattering angle ϑ between the vector $\mathbf{k}$ of the incoming wave and $\mathbf{k}'$ ($\mathbf{k}\cdot\mathbf{k}' = k_E^2\cos\vartheta$):

$$\psi^+_{\mathbf{k}}(\mathbf{x}) \approx \frac{1}{(2\pi)^{3/2}}\left[e^{i\mathbf{k}\cdot\mathbf{x}} + \frac{e^{ikr}}{r}f_k(\vartheta)\right], \qquad (17)$$

The comparison with (16) gives

$$\boxed{f_k(\vartheta) = -\frac{4\pi^2 m}{\hbar^2}\langle \mathbf{k}'|\hat T(E_k)|\mathbf{k}\rangle} \qquad (18)$$

The quantity $|f_k(\vartheta)|^2 d\Omega$ has the dimension of an area. It is the fraction of the flux of incoming particles that is scattered in $d\Omega$ at angle ϑ. This also offers the interpretation of the T-matrix.
A more physical picture of the scattering process requires the analysis in terms of wave-packets (see for example Weinberg).
The integral

$$\sigma(E_k) = 2\pi\int_0^\pi d\vartheta \sin\vartheta |f_k(\vartheta)|^2$$

is the **cross section**: it is the fraction of incoming flux that is scattered in any direction per unit time.

The identity (10) for the T-matrix becomes the **optical theorem**

$$\boxed{\mathrm{Im}\,\langle\mathbf{k}|\hat{T}(E_k)|\mathbf{k}\rangle = -\frac{\hbar^2 k}{16\pi^3 m}\sigma(E_k)} \tag{19}$$

In presence of many scatterers, randomly distributed with density n_S low enough that each scattering event is not affected by the potential of the other scatterers, the mean free path is $\ell_k = \frac{1}{\sigma(E_k)n_S}$.
Consider a cylinder with axis parallel to the particle's velocity, cross area A and length ℓ. It contains $n_s A\ell$ scatterers. The probability that the particle scatters is $(n_s A\ell)\sigma/A$. When the probability is 1, then ℓ is the mean free path.
The (inverse) scattering time is:

$$\boxed{\frac{1}{\tau(k)} = \frac{\hbar k}{m}\sigma(E_k)n_S} \tag{20}$$

Some useful links and references:

• J. R. Taylor, Scattering theory, the quantum theory of nonrelativistic collisions, Dover reprint.
• Rubin Landau, Quantum Mechanics II, John Wiley 1990.
• S. Weinberg, Lectures on Quantum Mechanics, Cambridge Univ. Press (2013).
• Amrein, Jauch, Sinha, Scattering theory in quantum mechanics, Benjamin 1977.
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• B. Zwiebach, Ch.7. Scattering (Quantum Physics III, MIT open courseware)
https://ocw.mit.edu/courses/physics/8-06-quantum-physics-iii-spring-2018/lecture-notes/MIT8_06S18ch7.pdf
• Maximilian Kreuzer, Ch.8 - Scattering theory, Vienna Tech. Univ.
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