Perturbation theory for scattering

We have derived the following equation for the scattering amplitude:

$$f(\mathbf{k}_i\mathbf{k}_f) = -\frac{1}{4\pi}\int e^{-i\mathbf{k}_f\mathbf{x}}v(\mathbf{x})\,\psi(\mathbf{x})\,d^3x \tag{1}$$

Here $\mathbf{k}_i$, $\mathbf{k}_f$ are the wave vectors of the incident and scattered waves; $v(\mathbf{x}) = \frac{2m}{\hbar^2}V(\mathbf{x})$, where $V(\mathbf{x})$ is the potential; $\psi(\mathbf{x})$ is the exact wave fuction of the particle whose incident plane wave is $e^{i\mathbf{k}_i\mathbf{x}}$. In the perturbation theory it is more convenient to employ the normalized plane wave states $|\mathbf{k}\rangle$ whose Schrödinger wave functions $\langle\mathbf{x}|\,\mathbf{k}\rangle = (2\pi)^{-3/2}\,e^{i\mathbf{k}\mathbf{x}}$ differ by a numerical factor from those used in eq. (1). Thus, the scatteing amplitude can be rewritten as a matrix element:

$$f(\mathbf{k}_i\mathbf{k}_f) = -\frac{(2\pi)^3}{4\pi}\langle\mathbf{k}_f|\,v\,|\psi_i\rangle\,, \tag{2}$$

where $|\psi_i\rangle$ is the state of scattering that has the state $|\mathbf{k}_i\rangle$ as its incident wave. The state $|\psi_i\rangle$ obeys the stationary Schrödinger equation $H|\psi_i\rangle = E\,|\psi_i\rangle$ with $H = H_0 + V$, where $H_0 = \frac{\mathbf{p}^2}{2m}$ is the kinetic energy, whereas $V = V(\mathbf{x})$ is the potential energy considered as perturbation. It can be rewritten as follows:

$$(E - H_0)\,|\psi_i\rangle = V\,|\psi_i\rangle \tag{3}$$

To any solution of this equation it is possible to add any solution of the equation $(E - H_0)\,|\psi_i\rangle = 0$, i.e. the vector of a free particle state, and the sum is also a solution of eq. (3). Therefore it is reasonable to transform the equation (3) as follows:

$$|\psi_i\rangle = |\mathbf{k}_i\rangle + (E - H_0 \pm i\delta)^{-1}\,V\,|\psi_i\rangle \tag{4}$$

Important! Here we added an infinitesimal imaginary term to the operator $E - H_0$ to make it regular at any real E. Otherwise at positive E, it nullifies all eigenstates of the Hamiltonian H_0 with energy equal to E and its inverse operator is not defined. We will see that the choice of the sign of imaginary constant is extremely substantial: positive sign corresponds to generation of the outgoing spherical wave by the potential, whereas the negative sign corresponds to generation of ingoing wave. Since the scattering is the generation of the outgoing waves by the satterer, we choose further the sign plus.

First of all we find matrix elements of the Green operator in momentum and coordinate representations. It is diagonal in the momentum or wave-vector representation, where the Hamiltonian is diagonal $\langle\mathbf{k}'|\,H_0\,|\mathbf{k}\rangle = \delta(\mathbf{k}-\mathbf{k}')\,\frac{\hbar^2\mathbf{k}^2}{2m}$. Therefore:

$$\langle\mathbf{k}'|\,G\,|\mathbf{k}\rangle = \frac{\delta(\mathbf{k}-\mathbf{k}')}{E - \frac{\hbar^2\mathbf{k}^2}{2m} + i\delta} \tag{5}$$

To find the same operator in coordinate representation we use the closure relations: $\langle\mathbf{x}'|\,G\,|\mathbf{x}\rangle = \int d^3k d^3k'\,\langle\mathbf{x}'|\,\mathbf{k}'\rangle\,\langle\mathbf{k}'|\,G\,|\mathbf{k}\rangle\,\langle\mathbf{k}|\,\mathbf{x}\rangle$. Emploing eq. (5) and

$\langle \mathbf{x} | \, \mathbf{k} \rangle = (2\pi)^{-3/2} \, e^{i\mathbf{k}\mathbf{x}}$, we arrive at the integral representation:

$$\langle \mathbf{x}' | \, G \, | \mathbf{x} \rangle = \frac{1}{(2\pi)^3} \int \frac{e^{i\mathbf{k}(\mathbf{x}'-\mathbf{x})} d^3k}{E - \frac{\hbar^2 \mathbf{k}^2}{2m} + i\delta} \tag{6}$$

The integration can be performed explicitly in terms of elementary functions. Let us introduce spherical coordinates in the wave-vector space directing the polar axis along the vector $\mathbf{x}' - \mathbf{x}$. Then the argument of exponent in nominator is equal to $k \, |\mathbf{x}' - \mathbf{x}| \cos \vartheta$ and $d^3k = k^2 dk \sin \vartheta d\vartheta d\varphi$. The integrand does not depend on φ, and the correponding integral gives a factor 2π. Integral of the exponent multiplied by $\sin \vartheta$ over ϑ is elementary and gives a factor $\frac{e^{ikR} - e^{-ikR}}{ikR}$, where $R = |\mathbf{x}' - \mathbf{x}|$. The remaining integral over k reads:

$$\langle \mathbf{x}' | \, G \, | \mathbf{x} \rangle = \frac{1}{(2\pi)^2 \, iR} \int_0^\infty \frac{\left(e^{ikR} - e^{-ikR}\right) k}{E - \frac{\hbar^2 k^2}{2m} + i\delta} dk \tag{7}$$

By the next step the two terms with e^{ikR} and e^{-ikR} in the integral (7) can be transformed into one integral from $-\infty$ to $+\infty$. Besides of that we extract a factor $\frac{2m}{\hbar^2}$ from the integral and denote $\frac{2mE}{\hbar^2} = k_0^2$. The transformed matrix element reads:

$$\langle \mathbf{x}' | \, G \, | \mathbf{x} \rangle = \frac{2m}{(2\pi)^2 \, iR\hbar^2} \int_{-\infty}^{\infty} \frac{e^{ikR} k dk}{k_0^2 - k^2 + i\delta} \tag{8}$$

This integral can be calculated by the method of Cauchy residue. The integrand has two simple poles at $k = \pm (k_0 + i\varepsilon)$, where ε is a positive infinitesimal value. Since e^{ikR} exponentially decreases in the upper half-plane of the complex variable k the contour of integration (the real axis of k) can be appended by the infinitely remote semicircle in the upper half-plane without changing the integral value. The resulting closed contour contains inside the pole in the upper half-plane $k = k_0 + i\varepsilon$. The residue of the integrand at this pole is equal to $-\frac{e^{ik_0 R}}{2}$. Thus, the final result is:

$$\langle \mathbf{x}' | \, G \, | \mathbf{x} \rangle = -\frac{2m}{\hbar^2} \frac{e^{ik_0 R}}{4\pi R} \tag{9}$$

This result differs from what we have found for the Green function of the Schrödinger equation for a free particle by a factor $\frac{2m}{\hbar^2}$. Simultaneously we have proved that the choice of positive sign at $i\delta$ in the Green function corresponds to the outgoing wave.

The solution of the equation (4) can be obtained by the method of consequent approximations over a small potential V. In zero approximation we neglect the term with the potential and obtain $|\psi_i\rangle_0 = |\mathbf{k}_i\rangle$. In the first approximation we substitute $|\psi_i\rangle_0$ in the last term in eq. (4) to get $|\psi_i\rangle_1 = |\mathbf{k}_i\rangle + GV \, |\mathbf{k}_i\rangle$. It is clear now that the n-th approximation to is $|\psi_i\rangle_n = \left[1 + (GV) + (GV)^2 + ... + (GV)^n\right] |\mathbf{k}_i\rangle$.

Returning to the equation (2) for the scattering amplitude, we get for the second Born approximation:

$$f_2\left(\mathbf{k}_i\mathbf{k}_f\right)=-\frac{(2\pi)^3}{4\pi}\frac{2m}{\hbar^2}\left[\left\langle\mathbf{k}_f\right|V\left|\mathbf{k}_i\right\rangle+\int\frac{\left\langle k_f\right|V\left|\mathbf{k}\right\rangle\left\langle\mathbf{k}\right|V\left|\mathbf{k}_i\right\rangle d^3k}{E-\frac{\hbar^2k^2}{2m}+i\delta}\right] \tag{10}$$

It looks much simpler in terms of the Fourier-components $v_{\mathbf{q}}=\int v\left(\mathbf{x}\right)e^{i\mathbf{qx}}d^3x$ of the reduced potential $v\left(\mathbf{x}\right)=\frac{2m}{\hbar^2}V\left(\mathbf{x}\right)$:

$$f_2\left(\mathbf{k}_i\mathbf{k}_f\right)=-\frac{1}{4\pi}\left(v_{\mathbf{k}_i-\mathbf{k}_f}+\int\frac{v_{\mathbf{k}_i-\mathbf{k}}v_{\mathbf{k}-\mathbf{k}_f}}{\mathbf{k}_i^2-\mathbf{k^2}+i\varepsilon}\frac{d^3k}{(2\pi)^3}\right) \tag{11}$$

The general term of the series in round brackets reads:

$$\int\frac{v_{\mathbf{k}_i-\mathbf{k}_1}v_{\mathbf{k}_1-\mathbf{k_2}}v_{\mathbf{k}_2-\mathbf{k_3}}...v_{\mathbf{k}_{\text{n-1}}-\mathbf{k}_f}d^3k_1...d^3k_{n-1}}{\left(\mathbf{k}_i^2-\mathbf{k_1^2}+i\varepsilon\right)\left(\mathbf{k}_i^2-\mathbf{k_2^2}+i\varepsilon\right)...\left(\mathbf{k}_i^2-\mathbf{k}_{n-1}^{\mathbf{2}}+i\varepsilon\right)(2\pi)^{3(n-1)}} \tag{12}$$

Note that this theory does not require spherical symmetry of the potential.