Coherent scattering in non relativistic quantum mechanics

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Abstract
In this paper we give a pedagogical explanation of coherence effects in non relativistic scattering processes. Coherent scattering is important not only because it is a clear manifestation of the wave character of the interaction in these regimes, but also because it helps in increasing the cross section and thus the observable effects. We show under which conditions a particle scatters coherently on a multi-particle system. In a nutshell, in order to have coherent scattering, the incident particle has not to resolve the internal structure of the composite system. We show that the above condition is satisfied when the de Broglie length of the incident particle is much larger than the size of the system.

Keywords: non relativistic scattering theory, coherent scattering, composite system scattering

1. Introduction

The aim of this paper is to study coherent scattering in the non relativistic regime. In general, when a particle is scattered by a composite system (e.g. an electron hitting an atom), the scattering depends in a non-trivial way on the interaction of the incident particle with each of the particles of the target. However, under certain conditions, all particles of the target scatter the incident particle in the same way, leading to ‘coherent scattering’.

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As we will show, coherent scattering arises when the incident particle does not resolve the internal structure of the target. In such a case, in first approximation, the target can be treated as a point-like object with total charge equal to the sum of the charges of its constituents\(^4\). Coherent scattering is interesting, for the following two properties: (i) it does not require a detailed knowledge of the internal structure of the target and (ii) when all the \(N\) constituents have the same charge, the cross section scales as \(N^2\) and, therefore, is larger compared to the case of incoherent scattering, where the cross section increase as \(N^\alpha\) with \(1 \leq \alpha < 2\) (\(\alpha = 1\) corresponds to the total incoherent scattering, where all the components of the target scatter independently, while for \(1 < \alpha < 2\) the scattering is partially coherent and partially incoherent).

Property (i) played a fundamental role on a very important and famous experiment of last century performed by Ernest Rutherford and his collaborators. They fired energetic \(\alpha\)-particles to foils of different materials, and measured the deflection of the scattered particles [1, 2]. From the distribution of scattered particles they deduced information on the structure of the foil and were able to prove the planetary model of the atom. The model used to fit the experimental data is very simple: the \(\alpha\)-particle and the nucleus are described as point-like particles and the details about their internal structure are ignored, exactly as in the coherent scattering regime. As a result, the cross-section scales with the square of the number of protons in the nucleus. This square dependence is a clear sign that all the protons in the nucleus scatter coherently off the incident \(\alpha\)-particle.

Property (ii) motivates our study on coherent scattering in the non-relativistic regime. In fact, different interferometry experiments in this regime have been recently proposed, where the interactions considered are usually very weak [3, 4]. Therefore, a quadratic increase of the cross section due to the presence of coherence may play an important role in making these experiments more effective.

The main result of this paper is to show under which conditions coherent scattering arises, i.e. when the De Broglie wave length of the incident particle is much larger than the typical size of the target. We focus on coherent scattering of matter waves. A similar analysis on coherent scattering of light is given in [5]. Moreover, an analysis on coherence phenomena in multiple scattering processes can be found in [6, 7].

The paper is organized as follows: in section 2 we study a simple model where a particle moving in one dimension is scattered by two Dirac delta potentials and we derive the conditions under which there is coherent scattering. In section 3 we repeat this analysis by studying, in the perturbative regime, a more realistic situation of scattering between a particle and a generic \(N\)-particle bound system, through a generic potential. Then we obtain the cross section in the coherent scattering regime. In section 4 we apply the coherent scattering cross section formula to the case of the scattering of \(\alpha\)-particle off nucleus of different atoms, re-obtaining the Rutherford cross section. To conclude, in section 5 we summarize the main results of the paper.

2. Coherent scattering: an exact calculation

We start our analysis by studying a simple model where all calculations can be carried out exactly. We consider the one dimensional scattering of a particle off two Dirac delta potentials. We start with this simple example in order to avoid unnecessary mathematical difficulties. We will get a clear picture of the conditions under which coherent scattering

\(^4\) We wish to clarify that, since the results we will obtain are general, here we refer to generic charges, not necessarily the electric charges
occurs. The dynamics of the system is described by the Schrödinger equation with Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \alpha \delta(\hat{x}) + \alpha \delta(\hat{x} - a),$$ \hspace{1cm} (1)

where $m$ is the mass of the particle and $\alpha$ is the coupling constant of the $\delta$-potentials (with dimension $[\alpha] = J \text{ m}$). As it is shown in appendix A, the scattering probability $R$ for this simple model is given by:

$$R = \frac{4[\beta \cos(ka) + \sin(ka)]^2}{2 + 2\beta^2 + \beta^4 + 2(\beta^2 - 1)\cos(2ka) + 4\beta \sin(2ka)},$$ \hspace{1cm} (2)

where $\beta = \frac{k^2a^2}{m^2}$ and $k$ is the wave vector of the incident plane wave. The scattering probability $R$ depends on $k$ and on the distance $a$ between the two delta potentials. We expect to observe coherent scattering when the particle’s wave length $2\pi/k$ is much larger than $a$ (which means $ka \ll 1$). In fact, in this regime, the distance between the two centers is small enough that the two scattered components of the wave come out with almost exactly the same phase, adding therefore coherently. In other words, the plane wave representing the incident particle does not resolve the distance $a$ between the two potentials and therefore it scatters off the two deltas as if they were one on top of the other. To verify this, let us approximate the reflection probability $R$ of equation (2) in the regime $ka \ll 1$. In this regime equation (2) becomes:

$$R \approx \frac{4}{4 + \beta^2} = \frac{1}{1 + \frac{k^2 \hbar^2}{m^2(2a)^2}}.$$ \hspace{1cm} (3)

This result should be compared with the reflection probability formula for a scattering process with only one delta potential in the origin:

$$R_{\text{single}} = \frac{1}{1 + \beta^2} = \frac{1}{1 + \frac{k^2 \hbar^2}{m^2a^2}}.$$ \hspace{1cm} (4)

We see that equation (3) describes the same reflectivity as that of a single delta with coupling constant $2\alpha$. In the regime $ka \ll 1$ the incident plane wave is not able to distinguish the two $\delta$-potential and their effect adds coherently.

Something interesting happens when the interaction is weak and perturbation theory can be applied. In the perturbative regime, the velocity of the particle is much larger than the coupling constant of the interaction i.e. $\frac{k \hbar}{m} \gg \frac{a}{\hbar}$, which is equivalent to having $\beta \gg 1$. Then the denominators in equations (3) and (4) can be approximated by $\beta^2$ and we have:

$$R \approx 4R_{\text{single}}.$$ \hspace{1cm} (5)

The factor 4 is exactly the contribution due to the presence of the two deltas. As we can see, when the Born approximation applies, the probability of having a scattering (which in this case is given by the reflectivity $R$) increases with the square of the number of the scattering centers. This, as we will show in the next sections, is true not only for this simple model, but also for more generic systems and interactions. Therefore, when the interaction is weak, the coherent scattering regime can be used to increase quadratically the cross section, and with it the measurable effects.
3. The scattering process

In this section we extend the previous results to a more generic situation: the scattering of a particle off a bound system of \( N \) particles (which in the following we will refer to this as ‘target’), in the non relativistic regime. We first define the target, the incident particle and the interaction.

3.1. The target

We consider a bound system of \( N \) interacting particles (e.g. an atom or a molecule), which is described by the following Hamiltonian:

\[
\hat{H}_0 = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m_i} + \sum_{i<j=1}^{N} \alpha_{ij} U(\hat{x}_i - \hat{x}_j), \tag{6}
\]

where \( \hat{q}_i \) is the momentum operator of the \( i \)th particle, \( \hat{x}_i \) its position operator, and the coupling constants \( \alpha_{ij} \) measure the strength of the interaction \( U \) between the \( i \)th and the \( j \)th particle. It is convenient to introduce the center of mass and relatives coordinates, which are given by:

\[
\begin{align*}
\text{Position of Center of Mass } \hat{X} &= \sum_{i=1}^{N} \frac{m_i}{M} \hat{x}_i, \\
\text{Total Momentum } \hat{P} &= \sum_{i=1}^{N} \hat{q}_i, \\
\text{Relative Positions } \left\{ \begin{array}{l}
\hat{r}_1 = \hat{x}_1 - \hat{X} , \\
\hat{r}_N = -\sum_{i=1}^{N-1} \frac{m_i}{m_N} \hat{r}_i ,
\end{array} \right.
\end{align*}
\tag{7}
\]

\[
\begin{align*}
\text{Relative Momenta } \left\{ \begin{array}{l}
\hat{p}_1 = \hat{q}_1 - \frac{m_1}{M} \hat{p}, \\
\hat{p}_N = -\sum_{i=1}^{N-1} \hat{p}_i,
\end{array} \right.
\end{align*}
\]

where \( i \in (1,...,N-1) \) and \( M = \sum_{i=1}^{N} m_i \) the total mass of the system. Using these coordinates, the Hamiltonian \( \hat{H}_0 \) of equation (6) can be written as

\[
\hat{H}_0 = \frac{\hat{P}^2}{2M} + \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m_i} + \sum_{i<j=1}^{N} \alpha_{ij} U(\hat{r}_i - \hat{r}_j), \tag{8}
\]

in which the separation between the center of mass degrees of freedom and the internal degrees of freedom is explicit.

3.2. Incident particle and interaction hamiltonian

We consider an incident particle with no internal structure, described by the free Hamiltonian \( \hat{H}_d \), which interacts with the target through interaction Hamiltonian \( \hat{H}_{int} \).
\[ \hat{H}_d = \frac{p_d^2}{2m_d}, \quad \hat{H}_{\text{int}} = \sum_{i=1}^{N} g_i V(\hat{\mathbf{Y}} - \hat{\mathbf{X}} - \hat{\mathbf{r}}_i). \]  

(9)

In the above equation \( g_i \) the coupling constants of the interaction between the incident particle and the \( i \)th particle of the target, \( \hat{\mathbf{Y}} \) the position operator of the incident particle and \( \hat{\mathbf{X}} \) and \( \hat{\mathbf{r}}_i \) are, respectively, the center of mass of the target and the relative coordinates of the \( i \)th particle, introduced above.

### 3.3. The scattering process

According to scattering theory [8, 9], the transition probability \( P_{\text{in} \rightarrow \text{out}} \) from an initial state \(|\text{In}\rangle\) to a final state \(|\text{Out}\rangle\) is given by [9]:

\[ P_{\text{in} \rightarrow \text{out}} = \left| \langle \text{Out} | \hat{T} | \text{In} \rangle \right|^2, \]  

(10)

where \( \hat{T} \) is the transition matrix defined via the scattering matrix as \( \hat{S} = 1 + \hat{T} \). The initial and final states \(|\text{In}\rangle\) and \(|\text{Out}\rangle\) are usually chosen to be eigenstates of the free Hamiltonian:

\[ |\text{In}\rangle = |p_d; \mathbf{P}; \phi\rangle, \quad |\text{Out}\rangle = |p'_d; \mathbf{P}; \phi'\rangle, \]  

(11)

where \( p_d \) is the momentum of the incident particle, \( \mathbf{P} \) the momentum associated to the center of mass of the target and \( \phi \) denotes an eigenstate of the Hamiltonian relative to the internal degrees of freedom of the target. Note that in this section we consider the initial state of the incident particle to be described by a plane wave. However, the extensions to the case of an incident particle described by a wave packet or the case of a beam of incident particles described by a statistical operator lead to very similar results. Appendices D and E contain an explicit calculation.

The transition probability \( P_{\text{in} \rightarrow \text{out}} \), computed in appendix B using standard perturbation theory, is:

\[ P_{\text{in} \rightarrow \text{out}} = \left| \left\langle p'_d, \mathbf{P}', \phi' \right| \hat{T} \left| p_d, \mathbf{P}, \phi \right\rangle \right|^2 = \frac{T}{(2\pi \hbar)^{2N}} \frac{\delta(E - E')}{\delta} \left( p_d + \mathbf{P} - p'_d - \mathbf{P}' \right) \]

\[ \times \left| \tilde{\mathbf{V}}(p_d - p'_d) \right|^2 \]

\[ \times \sum_{i=1}^{N} g_i g_i' \int d\{r\} \int d\{s\} e^{i\tilde{\mathbf{V}}(p_d - p'_d)(r - s)} \phi'(\{r\})^* \phi(\{s\}) \phi(\{s\})^* \phi'(\{r\}) \phi(\{s\}). \]  

(12)

where \( T \) is the time interval in which the scattering occurs, \( E \) and \( E' \) denotes, respectively, the total initial and final energy and \( \tilde{\mathbf{V}}(\mathbf{p}) \) the Fourier transform of the interaction potential \( V(\mathbf{x}) \). We also introduced the compact notation \(|\mathbf{r}\rangle = r_1, \ldots, r_{N-1} \) and \( \int d\{r\} = \prod_{i=1}^{N-1} \int dr_i \). From the last line of equation (12) we see that, in general, the contributions to the scattering probability given by each constituent of the target do not add coherently. However, there is a coherent effect when the contribution of each term is in phase with the others i.e. when we can approximate:

\[ e^{i\tilde{\mathbf{V}}(p_d - p'_d)(r - s)} \approx 1 \]  

(13)

in the second line of equation (12). Under this assumption and using the relation \( \int d\{r\} \phi'(\{r\})^* \phi(\{r\}) = \delta_{\phi',\phi} \), equation (12) becomes:
\[
P_{\text{in-out}} = \frac{T}{(2\pi \hbar)^3} \delta(E - E') \delta\left(\mathbf{p}_d + \mathbf{P} - \mathbf{p}'_d - \mathbf{P}'\right) \left| \mathbf{V} \left( \mathbf{p}_d - \mathbf{p}'_d \right) \right|^2 \left( \sum_{i=1}^{N} g_i \right)^2 \delta_{\phi, \phi'}, \quad (14)
\]

where \(\delta_{\phi, \phi'}\) implies that in this regime only scattering processes that do not excite the internal structure of the target are allowed.

Except for the delta and for the sum of the charges of the constituents there is no dependency on the internal structure of the target: the whole target behaves as a point-like object with total charge \(G = \sum_{i=1}^{N} g_i\). The coherent scattering given by condition equation (13) is equivalent to requiring \(\left|\mathbf{p}_d - \mathbf{p}'_d\right| r_i - s_j \ll \hbar\). This means that on the one hand, the binding potential \(U\) of the target must be strong enough to guarantee that the distances between its constituents are not too large; on the other hand the exchanged momentum \(\left|\mathbf{p}_d - \mathbf{p}'_d\right|\) should not be too large. However, \(\left|\mathbf{p}_d - \mathbf{p}'_d\right|\) is constrained by the conservation of momentum and energy contained in the two deltas in equation (14). This can be better seen by introducing the center of mass \(\mathbf{p}_s\) and relative coordinates \(\mathbf{p}_r\) of the whole system:

\[
\mathbf{p}_s = \mathbf{P} + \mathbf{p}_d, \quad \mathbf{p}_r = \frac{\mathbf{p}_d M - \mathbf{p}_d m_d}{m_d + M},
\]

and by noticing that, in the new coordinates, the two deltas can be written as:

\[
\delta(E - E') = \delta\left(\frac{\mathbf{p}_r^2}{2m_s} + \frac{\mathbf{p}_r^2}{2m_s}\right), \quad \delta\left(\mathbf{p}_d + \mathbf{P} - \mathbf{p}'_d - \mathbf{P}'\right) = \delta\left(\mathbf{p}_s - \mathbf{p}'_s\right),
\]

where \(m_s^{-1} = (M^{-1} + m_d^{-1})\) is the relative mass and \(m_s = M + m_d\) is the total mass. Using the restrictions given in equation (16) together with the relations in equation (15) we obtain:

\[
\left|\mathbf{p}_d - \mathbf{p}'_d\right| = \left|\mathbf{p}_r - \mathbf{p}'_r\right|, \quad \left|\mathbf{p}_r\right| = \left|\mathbf{p}'_r\right|,
\]

which gives the following bound for \(\left|\mathbf{p}_d - \mathbf{p}'_d\right|\):

\[
\left|\mathbf{p}_d - \mathbf{p}'_d\right| \leq 2 \left|\mathbf{p}_r\right|.
\]

Given the above results, the coherent scattering regime in equation (13) is fulfilled when

\[
\left|r_i - s_j\right| \ll \frac{\hbar}{2 \left|\mathbf{p}_s\right|},
\]

which means that the distance between the constituents of the target must be much smaller than the de Broglie wave length of the incident particle. This is in agreement with the result found for the simpler model discussed in section 2.

3.4. The coherent cross section

To conclude this section we compute the cross section in the coherent scattering regime. The starting point is the total cross section formula, defined as follow [10]:

\[
\sigma_{\text{tot}} = \frac{1}{n_{\text{inc}}} \sum_{\phi} \int \frac{dP_{\text{in-out}}}{dT} n\left(\mathbf{p}'_d\right) n\left(\mathbf{P}'\right) d\mathbf{p}'_d d\mathbf{P}',
\]

\[5\] Note that \(\mathbf{P}\) defined in equation (7) is the momentum of the center of mass of the target alone, while now we have introduced \(\mathbf{p}_s\), the momentum of the center of mass of the whole system, the target plus the incident particle.
where \( n(p') = n(P) = \frac{(2\pi\hbar)^3}{\int d\mathbf{x}} \) are the density of states, which we need to include because we are using plane waves in Dirac normalization and \( n_{\text{inc}} \) the incident flux of particles. Since we are interested in the coherent scattering cross section, the transition probability \( P_{\text{in} \rightarrow \text{out}} \) is the one given in equation (14). Note that in the coherent scattering regime the scattering probability does not depend on the internal state \( \phi(r) \). This is expected because, as already discussed, in this regime the incident particle does not resolve the internal structure of the target. The calculation, reported in appendix C, gives the result:

\[
\sigma_{\text{tot}} = m_r^2 \left( \sum_{i=1}^{N} g_i \right)^2 \int_{-1}^{1} d(\cos \theta) \left| \tilde{V} \left( \sqrt{8m_rE_r} \sin (\theta/2) \right) \right|^2, \tag{21}
\]

where \( E_r = p_r^2/2m_r \) with \( p_r \) the relative momentum defined in equation (15) and \( m_r \) the relative mass defined just after equation (16) and \( \theta \) is the scattering angle. The corresponding differential cross section is:

\[
\frac{d\sigma_{\text{tot}}}{d(\cos \theta)} = \left( \sum_{i=1}^{N} g_i \right)^2 \frac{m_r^2}{2\pi\hbar^4} \left| \tilde{V} \left( \sqrt{8m_rE_r} \sin (\theta/2) \right) \right|^2. \tag{22}
\]

As already discussed in the previous sections, the cross section in equation (22) depends on the total charge of the target \( G = \sum_{i=1}^{N} g_i \). In particular, when all the \( N \) constituents of the target have the same charge, i.e. \( g_i = g \) \( \forall i \), the cross section increases quadratically with \( N \).

4. Rutherford scattering

In Rutherford’s experiment, \( \alpha \) particles were fired to a thin foil of different materials and the angular distribution of the scattered particle was measured. The experiments showed clearly that there is a non negligible probability for the \( \alpha \) particles of being scattered at big angles. These observations led Rutherford to suggest the planetary model of the atom. The connection between Rutherford scattering and coherent scattering is that, in order to fit the experimental data with his model, Rutherford treated both the \( \alpha \) particles and the nucleus of atoms as point like objects, without considering the details of their internal structure. Therefore, in Rutherford scattering, all the protons of a nucleus scatter coherently the incident \( \alpha \) particle.

We now derive the Rutherford cross section starting from the coherent cross section of equation (22). The interaction is described by the Coulomb potential \( V(x) = 1/|x| \) and its Fourier transform is:

\[
\tilde{V}(p_r - p_r') = \int d\mathbf{x} \frac{\mathbf{e}^i(p_r - p_r') \cdot \mathbf{x}}{|\mathbf{x}|} = 4\pi\hbar^2 \frac{(p_r - p_r')^2}{|p_r|^2 + |p_r'|^2 - 2|p_r'| |p_r| \cos \theta} = \frac{4\pi\hbar^2}{m_rE_r (1 - \cos \theta)} = \frac{\pi\hbar^2}{2m_rE_r \sin^2(\theta/2)}, \tag{23}
\]

where, in the second line, we used \( |p_r| = |p_r'| \). With the help of equation (23) we can rewrite equation (22) as follows:
In equation (25) $\epsilon_0$ is the vacuum permittivity, $q_d = 2e$ is the charge of the $\alpha$ particles and $q_i = e$ are the charges of the protons of the nucleus. Since $i$ labels the different protons of the nucleus, then $i = 1, 2, \ldots Z$. Therefore we obtain:

$$\frac{d\sigma_{\text{tot}}}{d(\cos \theta)} = \frac{Z^2 e^2}{32\pi \epsilon_0 E_r^2 \sin^4(\theta/2)}.$$  \hspace{1cm} (26)

Since the mass of the $\alpha$ particle is much smaller than that of the nucleus, we can approximate $E_r \approx E_a$ and $\theta \approx \theta_a$ where $E_a$ and $\theta_a$ denote, respectively, the energy and the scattering angle of the incident $\alpha$ particle. Then equation (26) becomes:

$$\frac{d\sigma_{\text{tot}}}{d(\cos \theta_a)} = \frac{Z^2 e^2}{32\pi \epsilon_0 E_a^2 \sin^4(\theta_a/2)}.$$  \hspace{1cm} (27)

which is the Rutherford cross section. Because of the coherence of the scattering process, the cross section is proportional to the square of the number of protons of each nucleus\(^6\). This dependence has been observed experimentally by Rutherford and his collaborators [1, 2]. In their experiments, they measured the number of scintillations per minute in their detector, which is proportional to the number of $\alpha$ particles scattered per minute. Therefore, according to equation (27), when the experiment is repeated with different materials one should expect the quantity $N/Z^2$ to be constant. However, there is an additional effect, which must be taken into account: when an $\alpha$ particle goes through the material it can also be absorbed. In such a case the $\alpha$ particle is not detected. Bragg and his collaborators showed that the thickness of

\[^6\text{In the original paper of Rutherford [2] it was supposed that the total cross section was proportional to } A^2 \text{ instead of } Z^2. \text{ This is due to the fact that at the time when Rutherford performed the experiment, the existence of neutrons was not known. However, since now we know that only protons interact electromagnetically with the } \alpha \text{ particles, the cross section is proportional only to the square of the number of protons } Z.\]
the layer an \( \alpha \) particle can go through without being absorbed, goes as the inverse of the square root of the mass number \( A \). Therefore, when making the comparison with experimental data, also this effect must be included. In such a case the quantity \( N \sqrt{A/Z^2} \) is expected to be constant. The results of this analysis is reported in table 1. From the last column of the table we see that, apart for aluminum, for all the others materials we obtain values which are similar, as expected.

5. Conclusions

In this paper we have explicitly shown that a sufficient condition for coherent scattering is:

\[ \lambda_r \gg L, \quad (28) \]

with \( \lambda_r \) the de Broglie wave-length associated to the incident particle, as seen in the reference frame of the target, and \( L \) the typical spatial extension of the target. In this regime, the differential cross section in Born approximation is given by equation (22):

\[ \frac{d\sigma_{\text{tot}}}{d(\cos \theta)} = \left( \sum_{i=1}^{N} g_i \right)^2 \frac{m_e^2}{2 \pi \hbar^4} \left| \mathcal{V} \left( \sqrt{8m_r E_r \sin(\theta/2)} \right) \right|^2, \quad (29) \]

where the coherent effects are embedded in the dependence of the cross section on the square of the total charge \( G = \sum_{i=1}^{N} g_i \).

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Appendix A. One dimensional 2-delta potential scattering

In this appendix we show explicitly how to derive the reflectivity \( R \) of equation (2). We first solve the equation for the stationary states:

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \alpha [\delta(x) + \delta(x-a)] \psi(x) = E \psi(x) \quad (30) \]

associated to the Hamiltonian in equation (1), where \( m \) is the mass of the particle and \( \alpha \) is the coupling constant of the \( \delta \)-potential (with dimensions \( [\alpha] = J/m \)). To solve equation (30), we divide the \( x \)-axis in three regions: region ‘1’ with \( x \in (-\infty, 0) \), which is the region on the left of the first delta, region ‘2’ with \( x \in (0, a) \), which is the region between the two deltas and region ‘3’ with \( x \in (a, \infty) \), which is the region on the right of both deltas. We compute the reflection probability of a wave packet, coming from the left, which scatters off the delta potentials. Following the same procedure used in [11] \(^7\), it can

\(^7\) In [11] the calculation with a wave packet is performed for a square well potential. However the reasoning there is valid also for the problem we are considering.
been shown that the reflection probability can be computed by working with plane waves instead of considering wave packets. For each region we introduce the corresponding plane wave solutions of the free Schrödinger equation, \( \psi_j(x) \) with \( j = 1, 2, 3 \), which have the form:

\[
\psi_j(x) = c_j e^{ikx} + d_j e^{-ikx} \quad \text{with} \quad k = \frac{\sqrt{2mE}}{\hbar}.
\]  

(31)

The reflection probability is given by

\[
R := |d_1|^2/|c_1|^2,
\]

(32)

therefore we need to determine only the coefficients \( c_j \) and \( d_j \). This is done by using the following constrains imposed on the wave function \( \psi(x) \) by the Dirac-delta potentials.

1. The wave function must be continuous at the origin and at the point \( a \), i.e.:

\[
\psi_1(0) = \psi_2(0) \quad \text{and} \quad \psi_1(a) = \psi_2(a).
\]

(33)

2. Given a Dirac delta potential at a point \( a \), the right and left derivatives of the wave function at that point must obey the constraint:

\[
\psi'_L(a) - \psi'_R(a) = \frac{2ma}{\hbar^2} \psi_L(a),
\]

(34)

where \( \psi'_{RL}(x) := \frac{d}{dx} \psi_{RL}(x) \). In our case this corresponds to the following condition at the origin:

\[
\psi'_2(0) - \psi'_1(0) = \frac{2ma}{\hbar^2} \psi_1(0)
\]

(35)

and around the point \( a \):

\[
\psi'_j(a) - \psi'_j(a) = \frac{2ma}{\hbar^2} \psi_j(a).
\]

(36)

Equations (33), (35) and (36) set four conditions on the wave function \( \psi(x) \). Since, \( \psi(x) \) depends on the six parameters \( c_j \) and \( d_j \) (\( j = 1, 2, 3 \)), we still have two degrees of freedom. However, because we are considering particles coming from the left, and \( |c_1|^2 \) and \( |d_3|^2 \) give, respectively, the flux of incoming particles from the left and from the right, we can set \( c_1 = 1 \) and \( d_3 = 0 \).

Therefore we have:

\[
\psi_1(x) = e^{ikx} + d_1 e^{-ikx}, \quad \psi_2(x) = c_2 e^{ikx} + d_2 e^{-ikx}, \quad \psi_3(x) = c_3 e^{ikx}.
\]

(37)

Using the conditions given in equations (33), (35) and (36) we get:

\[
d_2 = -\frac{i \beta e^{2ika}}{e^{2ika} + 2i \beta + \beta^2 - 1},
\]

(38)

\[
c_2 = \frac{\beta (i + \beta)}{e^{2ika} + 2i \beta + \beta^2 - 1},
\]

(39)

\[
d_1 = -\frac{-1 + i \beta + e^{2ika}(1 + i \beta)}{e^{2ika} + (i + \beta)^2}.
\]

(40)
\[ c_3 = c_2 + d_2 e^{-2i\omega s}. \]  \hspace{1cm} (41)

where we introduced \( \beta = \frac{\hbar^2}{m a} \). Using the definition of reflection probability \( R \) given in equation (32) together with equation (40) and keeping into account that \( c_1 = 1 \), we obtain the result reported in equation (2).

**Appendix B. Perturbative calculation of transition probability**

In this appendix we derive the transition probability equation (12) by using perturbation theory.

We start by computing the transition amplitude \(<\text{Out} | \hat{T} | \text{In}>\), where the initial and final states are defined in equation (11) and

\[
\hat{T} = \hat{S} - 1 = \lim_{T \to \infty} \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{-T}^{+T} d\tau_1 \cdots \int_{-T}^{+T} d\tau_n \left\{ \hat{H}_I(\tau_1) \cdots \hat{H}_I(\tau_n) \right\}. \hspace{1cm} (42)
\]

where \( \hat{S} \) denotes the time ordering and \( \hat{H}_I \) is the potential introduced in equation (9) in the interaction picture. When the interaction is weak, we can stop the expansion at the first perturbative order (Born approximation) and \( \hat{T} \) becomes:\footnote{In order to use the Born approximation, we must be in the perturbative regime. This is true when \( \frac{\sqrt{E-E'}}{\pi} \ll \frac{1}{\hbar} \frac{1}{\sqrt{2E}} \), where \( R \) is the linear distance in which the potential is appreciably different from zero, \( \bar{V} \) is the mean potential in this region and \( p_r \) and \( m_r \), respectively, the relative momentum and mass between the target and the incident particle \[12\].}

\[
\hat{T} \approx \lim_{T \to \infty} -i \sum_{i=1}^{N} g_i \int_{-T}^{+T} d\tau \hat{V}_i \left( \hat{Y} - \hat{X} - \hat{r}_i ; \tau \right). \hspace{1cm} (43)
\]

where again the label ‘\( T \)’ denotes that we are taking the potential \( V(x) \) in the interaction picture.

The matrix element of the \( \hat{T} \) operator defined in equation (43) can be written as follows:

\[
\left\langle p'_d, P', \phi' \right| \hat{T} \left| p_d, P, \phi \right\rangle = \lim_{T \to \infty} -i \sum_{i=1}^{N} g_i \int_{-T}^{+T} d\tau e^{E+E' \tau} \int dY \frac{e^{i(P-P')\cdot Y}}{(2\pi\hbar)^3} \times \int dX \frac{e^{i(P-P')\cdot X}}{(2\pi\hbar)^3} \int d|r| V(Y - X - r_i) \phi'(|r|) \phi(|r|) = \lim_{T \to \infty} -i \int d[r] e^{i(P-p'_d)\cdot r} \phi'(|r|) \phi(|r|) \times \sum_{i=1}^{N} g_i \int d[r] e^{i(P-p'_d)\cdot r} \phi'(|r|) \phi(|r|) \hspace{1cm} (44)
\]

with \( E (E') \) the total initial (final) energy and where we introduced the compact notation \( |r| = r_1 \ldots r_{N-1} \) and \( \int d[r] = \prod_{i=1}^{N-1} \int d\tau_i \). In the third line we introduced the Fourier transform of the potential:

\[
\hat{V}(q) = \int dX e^{iq\cdot X} V(x), \hspace{1cm} (45)
\]
and the function $\delta_T(x)$, which is defined as follows:

$$\delta_T(x) = \frac{1}{2\pi \hbar} \int_{-T}^{T} dt \, e^{itx}, \quad \lim_{T \to \infty} \delta_T(x) = \delta(x). \tag{46}$$

It is worth pointing out the different meaning of the two delta functions in equation (44):

$$\delta\left(p_d + P - p'_d - P'\right), \quad \delta_T(E - E').$$

The first one implies that the scattering conserves the total momentum, the second one is a Dirac delta only when $T \to \infty$ and in this limit it implies the conservation of energy. Also, the following relations hold:

$$\lim_{T \to \infty} \delta_T(E) = \delta(0)\delta(E), \quad \delta(p)^2 = \delta(0)\delta(p) = \int_V \frac{dx}{(2\pi \hbar)^3} \delta(p), \tag{47}$$

where the integral over the volume appearing in the second term of equation (47) should be technically understood as over a very big but finite volume.

Inserting equation (44) in equation (10) and using the above relations, we obtain the scattering transition probability:

$$P_{\text{in}\to\text{out}} = \left| \left\langle p'_d, P', \phi' \right| \hat{T} \left| p_d, P, \phi \right\rangle \right|^2 = \frac{T}{2\pi \hbar} \int_V \frac{dx}{(2\pi \hbar)^3} \delta(E - E')$$

$$\times \delta\left(p_d + P - p'_d - P'\right) \left| \hat{V}(p_d - p'_d) \right|^2$$

$$\times \sum_{i,j=1}^N \delta_i \delta_j \int d\{r\} \int d\{s\} e^{i(\mathbf{p}_d - \mathbf{p}'_d)(\mathbf{r} - \mathbf{s})} \phi'([\mathbf{r}]) \phi([\mathbf{s}])^* \phi([\mathbf{s}]) \phi([\mathbf{s}])^*.$$

which is the formula for the transition probability equation (12).

**Appendix C. Calculation of the coherent scattering cross section**

In this appendix we compute the cross section in the coherent scattering regime. In order to do that we use the formula of coherent probability transition equation (14) in equation (20) and take into account that the incident flux of particles $n_{\text{inc}}$ is:

$$n_{\text{inc}} = \frac{1}{V} \int_V \frac{dx}{m_r} \tag{49}$$

where $p_r$ is the relative momentum introduced in equation (15) and $m_r$ the reduced mass defined just after equation (16). As result we get for the total cross section:

$$\sigma_{\text{tot}} = \frac{\left(\sum_{i=1}^{N} \delta_i \right)^2}{(2\pi)^2 \hbar^4} \int d\mathbf{p}_d \frac{d\mathbf{P}'}{dp_r} m_r \delta(E - E') \delta\left(p_d - p'_d + P - P'\right) \left| \hat{V}(\mathbf{P}' - \mathbf{P}) \right|^2. \tag{50}$$

It is convenient to introduce the center of mass $p'_s$ and the relative $p'_r$ final momenta:

$$\mathbf{P}'_s = \frac{\mathbf{P}'d M - \mathbf{P}'m_d}{m_d + M}, \quad \mathbf{P}'_r = \mathbf{P}' + \mathbf{P}'_d \tag{51}$$
so that equation (50) becomes:

\[
\sigma_{\text{tot}} = \frac{m_r}{|\mathbf{p}|} \left( \frac{\sum_{i=1}^{N} g_i}{(2\pi)^2 \hbar^4} \right)^2 \int d\mathbf{p}' \delta(E_r - E'_r) \left| \tilde{V}(\mathbf{p}_r - \mathbf{p}'_r) \right|^2, \\
\times \delta(\mathbf{p}_r - \mathbf{p}'_r) \left| \tilde{V} \left( \frac{M(\mathbf{p}'_r - \mathbf{p}_r)}{m_d + M} + \mathbf{p}_r - \mathbf{p}'_r \right) \right|^2,
\]

\[
= \frac{m_r}{|\mathbf{p}|} \left( \frac{\sum_{i=1}^{N} g_i}{(2\pi)^2 \hbar^4} \right)^2 \int d\mathbf{p}' \delta(E_r - E'_r) \left| \tilde{V}(\mathbf{p}_r - \mathbf{p}'_r) \right|^2, \\
= \frac{m_r^2}{\sqrt{E_r}} \left( \frac{\sum_{i=1}^{N} g_i}{(2\pi)^2 \hbar^4} \right)^2 \int d\Omega'_r \ dE'_r \sqrt{E'_r} \delta(E_r - E'_r) \left| \tilde{V} \left( \sqrt{2m_r E_r} \mathbf{n}_r - \sqrt{2m_r E'_r} \mathbf{n}'_r \right) \right|^2, \\
= \frac{m_r^2}{(2\pi)^2 \hbar^4} \left( \frac{\sum_{i=1}^{N} g_i}{(2\pi)^2 \hbar^4} \right)^2 \int d\Omega'_r \left| \tilde{V} \left( \sqrt{2m_r E_r} \mathbf{n}_r - \mathbf{n}'_r \right) \right|^2,
\]

\[(52)\]

where we introduced the unitary vectors \( \mathbf{n}_r := \mathbf{p}_r/|\mathbf{p}_r| \) and \( \mathbf{n}'_r := \mathbf{p}'_r/|\mathbf{p}'_r| \).

If the interaction potential depends only on the modulus of the relative distance, i.e. \( V(\mathbf{x}) = V(|\mathbf{x}|) \), then its Fourier transform depends only on the modulus of the transferred momentum \( \tilde{V}(|\mathbf{p}_r - \mathbf{p}'_r|) = \tilde{V}(|\mathbf{p}_r - \mathbf{p}'_r|) \). In such a case, we can write

\[
\left| \mathbf{n}_r - \mathbf{n}'_r \right| = \sqrt{n_r^2 + n'^2_r - 2 |\mathbf{n}_r| |\mathbf{n}'_r| \cos \theta} = \sqrt{2(1 - \cos \theta)} = 2 \sin(\theta/2),
\]

\[(53)\]

where \( \theta \) denotes the angle between \( \mathbf{n}_r \) and \( \mathbf{n}'_r \). Choosing a reference system where \( \mathbf{n}_r \) is oriented along the \( z \)-axis, we can rewrite \( d\Omega'_r = d\cos \theta dp \) and then obtain:

\[
\sigma_{\text{tot}} = m_r^2 \left( \frac{\sum_{i=1}^{N} g_i}{(2\pi)^2 \hbar^4} \right)^2 \int_0^{2\pi} \int_0^\pi dp \sin(\theta) \left| \tilde{V} \left( \sqrt{8m_r E_r} \sin(\theta/2) \right) \right|^2, \\
= m_r^2 \left( \frac{\sum_{i=1}^{N} g_i}{2\pi \hbar^4} \right)^2 \int_{-1}^1 \left( \cos \theta \right) \left| \tilde{V} \left( \sqrt{8m_r E_r} \sin(\theta/2) \right) \right|^2,
\]

\[(54)\]

which is the formula in equation (21).

**Appendix D. Wave packets instead of plane waves**

Here we extend the conditions for coherent scattering derived in section 3.3 by using plane waves, to the case where the initial state of the incident particle is a wave packet.

For the sake of simplicity, let us work in the reference frame where the target is at rest. Then the inequality in equation (19), which guarantees coherent scattering for plane waves, becomes:

\[
\left| \mathbf{p}_d \right| \ll L^{-1} \hbar,
\]

\[(55)\]

where \( L \) is the spatial extension of the target and \( \mathbf{p}_d \) is the momentum of the incident particle, before the scattering.
Now, instead of a plane wave with definite momentum, suppose we have a wave packet \( |\psi\rangle \). We expand it in the plane waves basis:

\[
|\psi\rangle = \int \hat{p}\psi(p)|p\rangle.
\]

(56)

In order to have coherent scattering, all plane waves composing the wave packet \( |\psi\rangle \) need to fulfill inequality (55). This is guaranteed when:

\[
|p_{\text{max}}| \ll L^{-1}\hbar.
\]

(57)

where \( p_{\text{max}} \) denotes the maximum significant momentum of the wave packet. For a wave packet with momentum average \( \langle \hat{p} \rangle_\psi \) and momentum spread \( \Delta p_\psi \), if we disregard the contributions coming from the tails of the momentum distribution \( \psi(p) \), we can approximate \( |p_{\text{max}}| \approx |\langle \hat{p} \rangle_\psi| + \Delta p_\psi \). Then the condition for coherent scattering becomes:

\[
|\langle \hat{p} \rangle_\psi| + \Delta p_\psi \ll L^{-1}\hbar
\]

(58)

or equivalently:

\[
\Delta x_\psi \gg L
\]

(59)

as one can easily prove with the help of the uncertainty principle.

**Appendix E. Ensembles of wave packets**

Now we consider the case of a incident beam of particles described by different wave packets. This beam is then described by a statistical mixture:

\[
\hat{\rho} = \sum_i \lambda_i |\psi_i\rangle \langle \psi_i|.
\]

(60)

ptwith \( \lambda_i \) are weights which sum to one, and \( |\psi_i\rangle \) are wave packets, each describing a single particle state. If all wave packets \( |\psi_i\rangle \) fulfill the coherent scattering condition (58), then the beam described by \( \hat{\rho} \) also describes coherent scattering, and verifies the following inequality:

\[
|\langle \hat{p} \rangle_\rho|^2 + (\Delta p_\rho)^2 \ll L^{-2}\hbar^2
\]

(61)

in fact:

\[
\Delta p_\rho^2 + \langle \hat{p} \rangle_\rho^2 = \text{Tr}[\hat{p}^2\hat{\rho}] = \sum_i \lambda_i \langle \hat{p}^2 \rangle_{\psi_i} = \sum_i \lambda_i \left[ (\Delta p_{\psi_i})^2 + \langle \hat{p} \rangle_{\psi_i}^2 \right]
\]

\[
\lesssim \hbar^2 L^{-2} \sum_i \lambda_i = \hbar^2 L^{-2}.
\]

(62)

Now the following apparent paradox appears. In general, an ensemble of ‘large enough’ wave packets (large with respect to \( L \), all of which scatter coherently, can be equivalently described by an ensemble of ‘small’ wave packets. Equivalent means that the two ensembles are associated to the same density matrix \( \hat{\rho} \). In particular, the second ensemble can be chosen in such a way that the size of the wave packets is small to the point that each incident particle sees only one constituent of the target. In such a case there cannot be coherent scattering. Here is the paradox: the two ensembles predict a different behavior for the scattering process, and this cannot be true, because they are equivalent and according to quantum theory they must give the same result. We clarify the situation. More specifically, we show that any \( \hat{\rho} \) which
satisfies the coherent scattering condition in equation (61) cannot be decomposed in terms of wave packets with spread in position smaller than $L$.

In fact, suppose that:

$$\hat{\rho} = \sum_i w_i |\phi_i\rangle \langle \phi_i|$$

such that every $|\phi_i\rangle$ satisfies: $\Delta x_{\phi_i} < L$. Then because of the uncertainty principle:

$$\Delta p_{\phi_i} > \hbar L^{-1}. \quad (64)$$

Of course this is in contrast with the coherent scattering condition (58). The important point is that, in this case, the statistical mixture $\hat{\rho}$ verifies the following inequality:

$$\langle \hat{\rho} \rangle^2 + \Delta p_{\hat{\rho}}^2 > \hbar^2 L^{-2} \quad (65)$$

as a simple computation similar to the one which brings from equation (61) to equation (62) shows. As we can see, conditions (61) and (65) are not compatible, meaning that the request of coherent scattering for $\hat{\rho}$ is incompatible with the request that the statistical operator can be decomposed in a mixture of wave functions $|\phi_i\rangle$, each of which is small enough to see only one scattering center.

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