Scattering of relativistic spinless particles within the Feshbach-Villars formalism

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A B S T R A C T

We consider the relativistic quantum scattering of spinless particles in one-spatial dimension using the Feshbach-Villars formalism. We construct the general form of the scattering matrix, for symmetric and non-symmetric potentials, based on the symmetry properties of the Feshbach-Villars equation. Then, since in one dimension there are only two partial waves associated with even and odd parities, we show, in a simple and comprehensive way, how to describe this transmission-reflection problem using partial-wave decomposition. As an illustration, we also discuss the special case of scattering by a symmetric square-well potential.

1. Introduction

The study of scattering processes, either involving relativistic or non-relativistic particles, has always been an active line of research. Indeed, these studies provide the standard tool to explore physical systems, whether being nuclear, atomic or solid state. Particularly, quantum scattering in one dimension (1D) has been attracting a great deal of attention [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]. As a matter of fact, understanding scattering effects in 1D is becoming increasingly important following latest advances in experimental realizations of mesoscopic systems and their promising applications in nanotechnology and quantum computing. This is, notably, in concordance with the study of tunnelling and transport phenomena in one-dimensional graphene superlattices [16, 17]. It has been also noted that quantum scattering in 1D is interesting for investigating the relation between Levinson’s theorem and the second virial coefficient for some physical systems [18]. But also, such a restriction to the one-dimensional case remains important from the pedagogical point of view. Indeed, it permits to significantly reduce the mathematical difficulty of the theory, but at the same time keeps sufficient physical complexity to elucidate the desired physical notions, such as the scattering matrix method or partial-wave decomposition and phases shifts. The latter occur in two and three dimensions and are known to be ubiquitous tools for handling scattering problems in quantum mechanics.

In the literature, there exist several works reporting, in comprehensive and pedagogical ways, on one-dimensional scattering in quantum mechanics and the related techniques for estimating different scattering properties. Notably, there is a large list of specific potentials for which exact analytic results are well known. Furthermore, as far as the scattering of relativistic spinless particles was concerned, the equation that has almost always been used is the Klein-Gordon (KG) equation. However, the latter is known to present some problems mainly related to the second derivative it contains. Actually, this equation cannot be viewed as an evolution equation like the Schrödinger equation. Indeed, the complete determination of the KG state at some time $t > 0$ requires knowing both the state and its time derivative at $t = 0$. Then, in order to get rid of this undesirable extra degree of freedom, Feshbach and Villars [19] suggested to reformulate the equation using a two-component wave function. This has led to an equation à la Schrödinger known as the Feshbach-Villars (FV) equation. However, compared to the that of KG, this equation has received relatively limited use in the study of scattering processes involving scalar bosons in relativistic quantum mechanics. This being said, it should nevertheless be pointed that a lot of works have been done around the FV equation, which has been considered within different contexts, including especially Klein paradox, pair production, and PT symmetric quantum mechanics (see for instance [20, 21, 22, 23, 24] and the references therein).

In this paper, we present a comprehensive discussion of the scattering problem of scalar bosons in 1D, within relativistic quantum me-
channics, using the FV representation. We show, in a simple manner, how such a problem can be handled by the methods of scattering matrix and partial-wave decomposition. We organize our paper as follows: in section 2 we review some well-known facts on FV formalism. In section 3 we derive the general form of the scattering matrix based on the symmetry properties of the FV equation. In section 4 we show how to handle the problem using partial-wave decomposition. We consider, first the special case of symmetric potential, then, we deal with the general case of non-symmetric potential. In section 5 we treat the special problem of scattering by a symmetric square well and we discuss, particularly, the low-momentum case. In the final section we give our conclusion.

2. Review of the Feshbach-Villars equation

First, we mention that throughout this paper we use natural units where \( \hbar = c = 1 \). The KG equation for a charged spin zero particle of mass \( m \) interacting with a four-vector potential \( A^\mu = (A_0, A) \) is given by

\[
(D_0 D^\mu + m^2) \Psi = 0 \tag{1}
\]

where \( D_0 \) is the minimally coupled derivative defined as \( D_0 = \partial_0 + i e A_0 \) with e the electric charge of the particle. One major drawback of the KG equation is that, because of being second order in time, the resulting density \( \rho_{KG} \) contains both \( \Psi \) and \( D_0 \Psi \) so that it is not possible to write \( \int \rho_{KG} d^3 x \) in the form \( \langle \Psi | \Psi \rangle = \langle \Psi | \Omega \Psi d^3 x \) with \( \Omega \) some matrix, and this implies the lost of the Hilbert space formalism [25]. As mentioned above, the second time derivative present in Eq. (1) indicates that \( \Psi \) has two degrees of freedom and not just one as for the Schrödinger equation. In order to emphasize this feature, Feshbach and Villars introduced a two-component column vector involving \( \Psi \) and its time-derivative [19]:

\[
\Phi \equiv \begin{pmatrix} \varphi \\ \chi \end{pmatrix} := \frac{1}{\sqrt{2}} \begin{pmatrix} \Psi + \frac{D_0}{m} \Psi \\ \Psi - \frac{D_0}{m} \Psi \end{pmatrix} \tag{2}
\]

so that Eq. (1) can be brought in the following Hamiltonian-form wave equation

\[
\frac{d\Phi}{dt} = H \Phi \tag{3}
\]

where \( H \) is a two \( \times \) two matrix Hamiltonian operator defined as

\[
H = \frac{\Pi^2}{2m} (\sigma_3 + i \sigma_2) + m_3 \sigma_3 + e A_0 I_2 \tag{4}
\]

Here \( \Pi \) is the gauge invariant momentum operator; \( \Pi = p - eA_1 I_2 \) refers to the 2 \( \times \) 2 unit matrix while \( \sigma_{1,2,3} \) are the usual Pauli’s matrices, but here they are acting in the vector space defined by Eq. (2) and not in the spin space. Eq. (3) is the so-called Feshbach-Villars (FV) equation. It is worth noting that the FV Hamiltonian defined above is pseudo-quasi hermitian in the sense that

\[
H^\dagger = \sigma_3 H \sigma_3. \tag{5}
\]

The density \( \rho \) and the current vector \( J \) associated with the FV equation are defined as follows [19]

\[
\rho = |\varphi|^2 - |\chi|^2 = \Phi \Phi^\dagger \\quad J = \frac{\Pi}{2m} \begin{pmatrix} \Phi \sigma_3 + i \sigma_2 \nabla \Phi - \nabla \Phi \sigma_3 + i \sigma_2 \Phi \\ -eA_0 \Phi \sigma_3 + i \sigma_2 \Phi \end{pmatrix} \tag{6}
\]

with \( \Phi = \Phi^\dagger \sigma_3 \). An apparent first advantage of using a two-component wave function is that the density \( \rho \) appears as the difference of two positive definite densities as might be expected in a formalism describing at the same time positive and negative charged particles. In this formalism \( \rho \) is indeed interpreted as a charge density, which by definition measures the difference between the number of positive and the number of negative particles. In this sense, the components \( \varphi \) and \( \chi \) can be then viewed as the relative weighting coefficients.

A second benefit of the two-component form of the wave function is to bring into focus the charge symmetry of the relativistic theory. This is easily seen by noting that the charge-conjugated wave function \( \Phi_\sigma \), which satisfies an equation similar to Eq. (3) but with the sign of the electric charge in \( H \) reversed, is given by

\[
\Phi_\sigma \equiv \sigma_3 \Phi^* = \begin{pmatrix} \chi^* \\ \varphi^* \end{pmatrix} \tag{7}
\]

where the star denotes the complex conjugate. Moreover, in the FV representation the Hilbert space formalism of the relativistic spin-zero theory, lost with the KG equation, is restored since the normalization of a state \( \Phi \) is given as

\[
\langle \Phi | \Phi \rangle = \int \Phi^\dagger \sigma_3 \Phi \ d^3 x = \pm 1 \tag{8}
\]

where solutions describing particles with opposite charges are oppositely normalized and this applies to \( \Phi \) and \( \Phi_\sigma \).

We end this section by noting that an eight-component equation, which is the spin-1/2 analogue of the above two-component FV equation has been constructed in [26, 27] by linearizing the time derivative in the Feynman-Gell-Mann equation [28], which is a relativistic equation for spin-1/2, alternative to the Dirac equation, but with a form comparable to the KG equation.

3. Scattering matrix in 1D

Consider a spin-0 particle subject to the potential \( V(x) \) in a 1D space. For a stationary state with energy \( E \), \( \Phi(t,x) = \chi(x) e^{-iE \tau} \), the FV equation reduces to the form

\[
\begin{pmatrix} (\sigma_3 + i \sigma_2) \frac{1}{2m} \frac{d^2}{dx^2} + m_3 + V(x) I_2 \end{pmatrix} \chi(x) = E \chi(x) \tag{9}
\]

We consider a real potential which vanishes sufficiently fast as \( |x| \to \infty \), so that \( \chi(x) \) becomes a free-particle state. We shall examine the transmission reflection problem in a general framework. Hence we assume the asymptotic wave function to be of the form

\[
\chi(x) = \begin{cases} \begin{pmatrix} A e^{ikx} + B e^{-ikx} \end{pmatrix} & \text{for } x \to -\infty \\ \begin{pmatrix} A'e^{ikx} + B'e^{-ikx} \end{pmatrix} & \text{for } x \to +\infty \end{cases} \tag{10}
\]

where \( k^2 = E^2 - m^2 \). \( A, B, A', B' \) are constant vectors of dimension 2. The incoming and the outgoing parts of the wave \( \chi(x) \) in the asymptotic region are

\[
\begin{align*}
\chi_{in}(x) &= A \theta(-x) e^{ikx} + B \theta(x) e^{-ikx} \\
\chi_{out}(x) &= A' \theta(x) e^{ikx} + B' \theta(-x) e^{-ikx}
\end{align*} \tag{11}
\]

where \( \theta(x) \) denotes the Heaviside function. Naturally, in the last equation, \( |x| \) is assumed to be much larger than the range of the potential. We define our scattering matrix \( S \) as the \( 4 \times 4 \) matrix relating \( \chi_{in}(x) \) to \( \chi_{out}(x) \) by

\[
\begin{pmatrix} A' \\ B' \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \tag{12}
\]

where the \( S_{ij} \) are bloc matrices of dimension \( 2 \times 2 \) forming together the matrix \( S \). If the potential vanishes, then \( A \to A' \) and \( B \to B' \) so that \( S \) reduces to the unit matrix. On the other hand, by considering the two special cases where either \( B'' = (0,0) \) or \( A'' = (0,0) \), where \( tr \) denotes the transpose operation, we can readily make from Eq. (12) the identification

\[
\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} T_L & R_R \\ T_R & R_L \end{pmatrix} \tag{13}
\]

where \( T \) and \( R \) are the transmission and reflection matrices, respectively. Suffix \( L \) \( (R) \) refers to the situation when the wave is incident from the left (from the right). In the following, we shall examine the different constraints satisfied by the bloc matrices \( S_{ij} \), which are, actually, not all independent. These constraints are derived from general conditions reflecting the symmetry of the FV equation.
a. The requirement of charge conservation; $\rho_{in} = \rho_{out}$, leads to the pseudo-unitarity of $S$:

$$\left(I_2 \otimes \sigma_z\right) S^\dagger \left(I_2 \otimes \sigma_z\right) = I_2,$$

where the symbol $\otimes$ designates the direct product of matrices.

b. Since there is no time dependence in the problem, the continuity equation $\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0$ implies that the current vector $\mathbf{j}$ is independent of $x$. Hence the flux of charge is expected to be continuous, that is:

$$\mathbf{J}_n = \mathbf{J}_{out},$$

which entails the condition

$$S^\dagger \left(I_2 \otimes \sigma_z\right) \left(I_2 \otimes \sigma_z\right) S = I_2.$$

c. For real potentials, the FV equation remains invariant under the time-reversal operation. This means that $\chi^*(x)$ is also a solution of Eq. (9). The vector $\chi^*(x)$ can be obtained from $\chi(x)$ given in Eq. (10) by making the substitutions $A \rightarrow B^\ast$ and $B \rightarrow A^\ast$. This leads to the condition

$$\left(I_2 \otimes \sigma_z\right) S^\dagger \left(I_2 \otimes \sigma_z\right) = S.$$

d. Since the mass of the particle appears in the K-G equation as $m^2$, the $S$-matrix must be invariant under the transformation $m \rightarrow -m$. The latter is equivalent to the substitution $\chi(x) \rightarrow \sigma_z \chi(x)$. This implies that

$$\left(I_2 \otimes \sigma_z\right) S \left(I_2 \otimes \sigma_z\right) = S.$$

e. For a symmetric potential, i.e., $V(x) = V(-x)$, $\chi(-x)$ is also a solution of Eq. (9). Since $\chi(-x)$ can be deduced from $\chi(x)$ by making the substitutions $A \rightarrow B$ and $A' \rightarrow B'$, we find that

$$(\sigma_1 \otimes I_2) S \left(\sigma_1 \otimes I_2\right) = S.$$ Combining all the previous properties, we obtain the following simplified forms of the bloc matrices $S_{ij}$:

- If $V(x)$ is non-symmetric:

$$S_{11} = S_{22} = \begin{pmatrix} t & 0 \\ 0 & \bar{t} \end{pmatrix}, \quad S_{12} = \begin{pmatrix} r & 0 \\ 0 & r \end{pmatrix}, \quad S_{21} = \begin{pmatrix} \rho & 0 \\ 0 & \rho \end{pmatrix}$$

where $t$, $r$, and $\rho$ are complex parameters which depend in general on the form of the potential. Moreover, from the pseudo-unitarity condition of $S$ we have

$$|t|^2 + |r|^2 = 1, \quad |t|^2 + |\rho|^2 = 1, \quad t^*r + \rho^*t = 0.$$  \hspace{1cm} (21)

- If $V(x)$ is symmetric:

$$S_{11} = S_{22} = \begin{pmatrix} t & 0 \\ 0 & t \end{pmatrix}, \quad S_{12} = S_{21} = \begin{pmatrix} r & 0 \\ 0 & r \end{pmatrix}$$

with the additional constraints

$$|t|^2 + |r|^2 = 1, \quad t^*r + r^*t = 0.$$  \hspace{1cm} (22)

At this level, it is worth to mention that the construction of the scattering matrix for the FV equation in 1D was previously considered in Ref. [29] where the form stated for $S$ was the same as the one found above. Yet, the authors of [29] did not evoke the arguments b. and d. and claimed that only conditions a., c. and e. had been used to get the result. However, we stress here the need of imposing all the constraints a.--e. in order to achieve the above form of the scattering matrix.

Next, by looking at $S$ we note that in both cases of symmetric and non-symmetric potentials we have $S_{11} = S_{22}$, i.e., $T_l = T_R$. Therefore, we will henceforth suppress the suffixes $L$ and $R$ of $T$. Moreover, we can remark that the scattering matrix has always the form

$$S = \begin{pmatrix} t & t \\ \rho & \rho \end{pmatrix}$$

with $\rho = r$ in the symmetric-potential case. This implies that $S$ does not mix the upper and the lower components of the FV wave function and, further, that these components are scattered in the same manner: for both components we can define a reduced scattering matrix $\mathcal{S}$ which is then given by

$$\mathcal{S} = \begin{pmatrix} t & t \\ \rho & \rho \end{pmatrix}$$

This form of $\mathcal{S}$, along with the relations (21), is the same as that of the scattering matrix in 1D obtained for the Schrödinger equation [5, 13] and also for the Dirac equation using the two-component approach [8]. This is natural since the physical arguments used for constructing the general form of the matrix $S$ are indeed the same.

It is worth noting that many authors prefer to describe the quantum scattering by means of the transfer matrix $M$ rather than the $S$ matrix because the former is more effective for studying coupled systems (see for instance [13] and references therein). By analogy with the non-relativistic case [13], we can define the matrix $M$ for the FV equation through the relation

$$\begin{pmatrix} A \\ B' \end{pmatrix} = M \begin{pmatrix} A' \\ B \end{pmatrix}$$

It is clear from this Eqs. (12) and (26) that $M$ and $S$ are not independent and, further, that their elements can be easily obtained from each others. Then, from Eq. (24) and with the help of Eq. (21) it is straightforward to show that

$$M = \begin{pmatrix} 1/t & r^*/t' \\ \rho/t & 1/r' \end{pmatrix} \otimes I_2$$

revealing again a great similarity in the form with the non-relativistic case [13].

At this stage, it is important to recall that if we consider only an incident wave from the left ($B = 0$), the transmission and reflection probabilities are given by the relations

$$T = |t|^2, \quad R = |r|^2$$

which can be easily verified by returning to the definitions:

$$T = \frac{|T_{\text{transmitted}}|^2}{|T_{\text{incident}}|^2}, \quad R = \frac{|T_{\text{reflected}}|^2}{|T_{\text{incident}}|^2}$$

and using the expression of $T$ given in Eq. (6).

We end this section with a comment on the behaviour of the elements of $S$, i.e., $t$, $r$ and $\rho$ as functions of $k$. To this end, let us designate the FV wave function by $\chi(k, x)$. As noted previously, $\chi^*(k, x)$ satisfies Eq. (9), but does not have the same asymptotic form as $\chi(k, x)$. On the other hand, $\chi^*(-k, x)$ is also a solution of Eq. (9) because, in the $k$-space, it depends precisely on $k^2$. Therefore $\chi^*(-k, x)$ and $\chi(k, x)$ have the same asymptotic form. This entails that

$$t^*(-k) = t(k), \quad r^*(-k) = r(k), \quad \rho^*(-k) = \rho(k)$$

Thus, in the threshold case, i.e., when $k \to 0$, each of the coefficients $t$, $r$ and $\rho$ should necessarily be real.

4. Partial-wave description

In this section, we shall rewrite the $S$-matrix in the partial-wave representation. In contrast to two and three-dimension situations where the number of partial waves is infinite, in one dimension, there are only two partial waves, one with even parity and the other with odd parity. Thus, we shall decompose our wave function as a sum of even and odd parity parts. This can be easily achieved by introducing new two-component vectors $C_0$ and $C_1$ which are related to $A$ and $B$ by the unitary transformation
\[
\begin{pmatrix}
\frac{C_0}{C_1}
\end{pmatrix}
= \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 \\
\mathrm{i} & \mathrm{i} \\
\end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}.
\] (31)

And we define two other vectors \(C'_0\) and \(C'_1\) related in an exactly similar manner to \(A\) and \(B\). Then, in terms of the new vectors, the incoming and the outgoing waves are now given by
\[
\chi_{\text{in}}(x) = \frac{1}{\sqrt{2}} \left[ C'_0 + \mathrm{i} \tau C'_1 \right] e^{-\mathrm{i} k|x|}, \quad \chi_{\text{out}}(x) = \frac{1}{\sqrt{2}} \left[ C'_0 - \mathrm{i} \tau C'_1 \right] e^{\mathrm{i} k|x|}
\] (32)

where \(\tau = x/\lambda\). In the partial-wave representation, the scattering matrix, that we shall denote by \(S\), is defined as
\[
\begin{pmatrix}
\frac{C'_0}{C'_1}
\end{pmatrix}
= S \begin{pmatrix}
\frac{C_0}{C_1}
\end{pmatrix}.
\] (33)

That being so, it is easy to show that \(S\) is related to \(S\) such that
\[
S = \frac{1}{2} \begin{pmatrix}
2 S_{11} + S_{12} + S_{21} & i (S_{12} - S_{21}) \\
 i (S_{12} - S_{21}) & 2 S_{11} - S_{12} - S_{21}
\end{pmatrix}
\] (34)

where we have used the property \(S_{11} = S_{22}\). Remark that \(S\) is a symmetric matrix.

### 4.1. Scattering by a symmetric potential

In the case of a symmetric potential, we have \(S_{12} = S_{21}\), i.e., \(R_L = R_R = R\), so that the matrix \(S\) becomes diagonal:
\[
S = \begin{pmatrix}
T + R & 0 \\
0 & T - R
\end{pmatrix} = \begin{pmatrix} t + r & 0 \\ 0 & t - r \end{pmatrix} \otimes \mathbf{I}_2.
\] (35)

which means that the two partial waves are decoupled. Note also that due to Eq. (23) the matrix \(S\) is unitary: \(S^* S = \mathbf{I}_4\). Furthermore, given the above form of \(S\), it is possible to rewire it as
\[
S = \begin{pmatrix}
e^{2\alpha_0} & 0 \\
0 & e^{2\alpha_1}\end{pmatrix} \otimes \mathbf{I}_2,
\] (36)

where \(\alpha_0\) and \(\alpha_1\) are two real phases having the arbitrariness of modulo \(\pi\). Subsequently, using Eqs. (32) and (36), the asymptotic form of the total wave function, sum of \(\chi_{\text{in}}\) and \(\chi_{\text{out}}\), can be reexpressed as
\[
\chi(x) \to \frac{1}{\sqrt{2}} \left[ \chi_0(x) C_0 + \chi_1(x) C_1 \right]
\] (37)

with
\[
\chi_i(x) = (\mathrm{i} \tau)^j \left[ e^{\mathrm{i} k|x|} + (-1)^j e^{2\mathrm{i} \alpha_j k|x|} \right]
\] (38)

that is,
\[
\chi_0 = 2 e^{\mathrm{i} \alpha_0} \cos \left( k |x| + \alpha_0 \right), \quad \chi_1 = 2 e^{\mathrm{i} \alpha_1} \sin \left( k |x| + \alpha_1 \right)
\] (39)

It is worth noting that this parametrization of the asymptotic FV wave function is very similar to that used for the Schrödinger wave function when defining partial-wave phase shifts in the context of non-relativistic quantum scattering in 1D Refs. [1, 5, 6]. In particular, the angle \(\alpha_j\) represents the scattering phase shift of the \(j^{th}\) wave.

Then, in the situation where an incident plane wave \(e^{\mathrm{i} k x}\) is coming from the left, the asymptotic form of the wave function \(\chi(x)\) can be written as
\[
\chi(x) \to \frac{1}{\sqrt{4\mathrm{m} E_0}} \left[ e^{\mathrm{i} k x} + f_+ e^{\mathrm{i} k|x|} \right] \begin{pmatrix} m + \mathrm{v} E_0 \\ m - \mathrm{v} E_0 \end{pmatrix}
\] (40)

where \(\tau = x/\lambda\), \(E_0 = \sqrt{k^2 + \mathrm{v}^2}\) is the scattered outgoing wave, \(f_+\) is the scattering amplitude and \(\mathrm{v}\) is the sign of the charge of the incident wave, that is \(\mathrm{v} = 1\) (\(\mathrm{v} = -1\)) for the scattering of “particles” ("antiparticles"). Hence, matching the coefficients of \(e^{\mathrm{i} k x}\) and \(e^{\mathrm{i} k|x|}\) in Eqs. (37) and (40), yields the results: 
\[
f_+ = \frac{1}{2} \left( e^{2\mathrm{i} \alpha_0} - 1 \right) = \mathrm{i} e^{\mathrm{i} \alpha_0} \sin \alpha_1, \quad \tau \to 0.1
\] (41)

The coefficients \(f_+\) and \(f_-\) are then the scattering amplitudes in the forward and the backward directions, respectively. For given phases \(\alpha_0\) and \(\alpha_1\), the parameters \(t\) and \(r\) can be obtained from the relations
\[
t = \frac{1}{2} \left( e^{2\mathrm{i} \alpha_0} + e^{2\mathrm{i} \alpha_1} \right), \quad r = \frac{1}{2} \left( e^{2\mathrm{i} \alpha_0} - e^{2\mathrm{i} \alpha_1} \right)
\] (42)

Note that \(t\) and \(r\) are related to \(f_+\) by
\[
t + f_+ = 1 + g_0 + g_1, \quad r = f_0 - g_1
\] (43)

In analogy with three-dimensional case, the discrete differential cross sections, in the forward and the backward directions, are given by 
\[
\sigma_+ = |f_+|^2, \quad \sigma_- = |f_-|^2
\] (44)

This expression is the same as that obtained for \(\sigma_+\) in the non-relativistic case [5, 6].

### 4.2. Non-symmetric potential

We assume now that \(V(x) \neq V(-x)\). In this case \(S_{12} \neq S_{21}\) so that the matrix \(S\) is no longer diagonal, then leading to a coupling of the two partial waves. Nevertheless, as will be shown below, it is still possible to diagonalize \(S\) through an appropriate pseudo-unitary transformation. To do so we define the matrix \(P\) as
\[
P = \begin{pmatrix}
\cos \alpha & -\sin \alpha \\
\sin \alpha & \cos \alpha
\end{pmatrix} \otimes \mathbf{I}_2.
\] (45)

where \(\alpha\) is a real parameter which will be fixed so that the transformed matrix \(S_D := P S P^*\) with \(U = (I \otimes \sigma_z) U^* (I \otimes \sigma_z)\), is diagonal. Then, we find
\[
S_D = \begin{pmatrix}
c^2 S_{11} + s^2 S_{22} + 2 s c S_{12} & c s (S_{22} - S_{11}) + (c^2 - s^2) S_{12} \\
-s s (S_{22} - S_{11}) + (c^2 - s^2) S_{12} & s^2 S_{11} + c^2 S_{22} - 2 s c S_{12}
\end{pmatrix}
\] (46)

where we have used the abbreviations \(c\) and \(s\) for \(\cos \alpha\) and \(\sin \alpha\), respectively. Hence, bearing in mind Eq. (20) and Eq. (34), it is straightforward to verify that \(S_D\) can be diagonalized by choosing \(\alpha\) as
\[
\tan(2\alpha) = \frac{r - \rho}{r + \rho},
\] (47)

which is also equivalent to the condition \(\rho = re^{\mathrm{i} \alpha}\). On the other hand, we can easily see from the first two relations in Eq. (21) that \(|r| = |\rho|\), which implies that \(\alpha\) should indeed be real. Therefore, we have an arbitrariness of modulo \(\pi\) in fixing the value of \(\alpha\). Then, with such a choice of \(\alpha\) the matrix \(S_D\) becomes
\[
S_D = \begin{pmatrix}
t + r e^{2\mathrm{i} \alpha} & 0 \\
0 & t - r e^{2\mathrm{i} \alpha}
\end{pmatrix} \otimes \mathbf{I}_2.
\] (48)

Moreover, using the third relation in Eq. (21) along with the relation \(\rho = re^{\mathrm{i} \alpha}\) we can easily show that \(|t + r e^{2\mathrm{i} \alpha}| = |t - r e^{2\mathrm{i} \alpha}| = 1\). Hence, the matrix \(S_D\) can be written as
\[
S_D = \begin{pmatrix}
e^{2\mathrm{i} \alpha_0} & 0 \\
0 & e^{2\mathrm{i} \alpha_1}\end{pmatrix} \otimes \mathbf{I}_2
\] (49)

with \(\alpha_0\) and \(\alpha_1\) real phases. Furthermore, since for \(a = 0\) the matrix \(S_D\) reduces exactly to that of the symmetric-potential case when the two partial waves are not mixed, we refer to \(a\) as the mixing parameter [2, 4]. The parameters \(\alpha_0\) and \(\alpha_1\) are called the eigenphases and they reduce to the phase shifts \(\alpha_0\) and \(\alpha_1\), respectively, for \(a = 0\).
The resulting form of the total asymptotic wave functions is given by

\[
\chi(x) \rightarrow \frac{1}{\sqrt{2}} \left[ Z_0(x) D_0 + Z_1(x) D_1 \right] 
\]

with

\[
Z_i(x) = (i\pi)^{\frac{3}{2}} \left[ e^{-i(k|x| - \varpi)} + (-1)^i e^{i2\varpi} e^{i(k|x| - \varpi)} \right]
\]
i.e.,

\[
Z_0 = 2e^{i\rho} \cos (k|x| - \varpi + \gamma_0), \quad Z_1 = 2e^{i\rho} \sin (k|x| - \varpi + \gamma_1)
\]

Next, let us obtain \(r, \rho\) and \(\varphi\) from given \(\gamma_0, \gamma_1\) and \(\alpha\). By identifying Eq. (47) and Eq. (48), it can be easily seen that

\[
t = \frac{1}{2} (e^{2i\rho} - e^{-2i\rho})
\]

while

\[
r = \frac{1}{2} (e^{2i\rho} - e^{-2i\rho}) e^{-2i\rho} - \frac{1}{2} (e^{2i\rho} - e^{-2i\rho}) e^{2i\rho}
\]

We end this section by looking at the scattering cross section. Again we assume an incident wave coming from the left. It can be easily verified that the relation between \(t, \rho\) and the scattering amplitudes \(f_i\) is still given by Eq. (43) with \(r\) replaced by \(\rho\). Then the total scattering cross section is given by

\[
\sigma_i = 2 (\sin^2 \gamma_0 + \sin^2 \gamma_1) = |t - 1|^2 + |\rho|^2
\]

The \(\sigma_i\) does not explicitly depend on the mixing parameter \(\alpha\), neither on the direction of the incident wave: for an incident wave from the right, we have just to replace \(\rho\) by \(r\). Of course \(\gamma_0\) and \(\gamma_1\) are not changed in this case.

5. Scattering by a square well

In this section we study the scattering of free particles by a symmetric square well potential of depth \(V_0\) and width 2\(\alpha\):

\[
V(x) = V_0 \theta(a - |x|)
\]

with \(V_0 < 0\). Thus, we have to solve the stationary FV equation

\[
\left[ -\frac{1}{2m} \frac{d^2}{dx^2} + (\sigma_1 + \sigma_2) + m\sigma_1 + V(x) - E \right] \phi_1(x) = 0
\]

in the three regions: region 1 for \(x \leq -a\), region 2 where \(-a \leq x \leq a\) and region 3 for \(x \geq a\). Then, defining a new column vector \(\varphi := \sqrt{2} (\sigma_1 + \sigma_2) \chi\), it is straightforward to verify that the upper component of \(\varphi\); \(\varphi_1\), satisfies the KG equation

\[
\frac{d^2}{dx^2} + (E - V(x)) \varphi_1(x) = 0
\]

while the lower component; \(\varphi_2\), can be simply obtained from \(\varphi_1\) using the relation \(\varphi_2 = (E - V)\varphi_1/m\). The function \(\varphi_1(x)\) in the first region is thus given by

\[
\varphi_1(x) = b_1 e^{ikx} + b_2 e^{-ikx}
\]

where \(b_1\) and \(b_2\) are constants, while \(k\) is the particle wave number outside the barrier: \(k = \sqrt{E - m^2}\). In the two remaining regions, \(\varphi_1(x)\) is also given by Eq. (50) with \(b_1\) and \(b_2\) respectively replaced by \(b_1\) and \(b_2\) in region 3, while in region 2 \(b_1\) and \(b_2\) and \(k\) are replaced respectively by \(c_1\) and \(c_2\) and \(k_1\), where \(k_1\) is the particle wave number within the barrier: \(k_1 = \sqrt{(E - V_0^2)/m^2}\).

Furthermore, since \(\varphi_1(x)\) is just the KG function, it satisfies the naive boundary conditions, i.e., \(\varphi_1(x)\) and its derivative are continuous at \(x = -a\) and \(x = a\). This leads to

\[
b_1 = (c_1 - i\xi s_1) e^{i\kappa_1 d_1} + i\xi s_1 d_2
\]

with the abbreviations \(c_1 = \cos (2k_1 a)\) and \(s_1 = \sin (2k_1 a)\) and the auxiliary notations:

\[
\xi = \frac{k^2 + k_1^2}{2k_1}, \quad \zeta = \frac{k^2 - k_1^2}{2k_1}
\]

Then, the asymptotic FV wave functions at \(x \rightarrow \pm \infty\) are indeed those of region 1 and region 3, which are given by

\[
\chi(x) = \frac{1}{\sqrt{2}} \left( \frac{m E}{\alpha^2 k_1} \right) \left( b_1 e^{ikx} + b_2 e^{-ikx} \right)
\]

for region 1 and the same for region 3 with \(b_1\) and \(b_2\) replaced by \(d_1\) and \(d_2\), respectively. Then, in order to exploit the properties of the S-matrix derived in section 3, we compare our asymptotic wave functions with Eq. (10) and we use Eq. (12) to infer that the constants \(b_1, d_1\) and \(d_2\) are related to the coefficients \(t\) and \(r\) as

\[
b_1 = \frac{1}{t} d_1 - \frac{r}{t} d_2
\]

By identification with Eq. (59) we obtain the following expressions for \(t\) and \(r\)

\[
t = e^{-2ik_1} \frac{c_1 - i\xi s_1}{c_1 - i\xi s_1}, \quad r = -i \frac{\zeta c_1 e^{-2ik_1}}{\zeta c_1 e^{-2ik_1}}
\]

and we can easily see that the conditions \(r(-k) = r(k)\) and \(r(-k) = r(k)\), proven in section 3, are well satisfied in this case. Subsequently, for the transmission and reflection probabilities a distinction should be made between two different situations: \(k_1^2 > 0\) and \(k_1^2 < 0\). For \(k_1^2 > 0\), i.e., \(k_1\) is real we obtain

\[
T = \frac{1}{1 + \zeta^2 s_1^2}, \quad R = \frac{\zeta^2 s_1^2}{1 + \zeta^2 s_1^2}
\]

whereas, for \(k_1^2 < 0\), i.e. \(k_1\) is purely imaginary, by setting \(k_1 = i k_2\) we find

\[
T = \frac{1}{1 + s_1^2 s_2^2}, \quad R = \frac{s_1^2 s_2^2}{1 + s_1^2 s_2^2}
\]

with

\[
\xi = \frac{k_1^2 + k_2^2}{2k_2}, \quad c_2 = \cos (2k_2 a), \quad s_2 = \sin (2k_2 a)
\]

Remark that for the two cases \(T\) and \(R\) satisfy the balance equation \(T + R = 1\). Note that the phase shifts can be easily calculated from Eq. (62) and Eq. (42).

For a more quantitative analysis, we plot in Fig. 1 the coefficients \(T\) and \(R\) as functions of the energy of the incident wave. We can see that, as \(E\) increases from zero, the transmission probability increases from zero to one then carries out continuous oscillations before stabilizing at around one. Conversely, the reflection probability decreases from one to zero, oscillates then tends to stabilize at nearly zero.

We also show in Fig. 2 the variations of the phase shifts with the well depth for fixed energy. We see that, in the considered energy range, \(\delta_0\) and \(\delta_1\) have almost sawtooth-like curves.

Next, let us examine the threshold case for the square-well potential. Assume for the moment that \(k_1^2 > 0\). According to Eqs. (62) we have, a priori, the threshold values \((t, r) = (0, -1)\) and therefore \((\delta_0, \delta_1) = (\pi/2, 0)\) modulo \(\pi\). This means that an incident wave with \(k \rightarrow 0\) is normally totally reflected by the square well. However, as for the scattering of Dirac particles [8], this situation will be completely turned on if the scattering potential supports a half bound state, i.e., a state with an energy \(E = m\) or \(E = -m\). In that case, one of the two following cases can occur: either \((t, r) = (1, 0)\) and \((\delta_0, \delta_1) = (0, 0)\) (situation 1), or \((t, r) = (-1, 0)\) and \((\delta_0, \delta_1) = (\pi/2, \pi/2)\) (situation 2). And notice that in both cases the incident wave is totally transmitted. As a matter of fact, the bound spectrum of the square well can be easily obtained: there are
Fig. 1. The Transmission and reflection coefficients as functions of the energy $E$ for fixed well depth and width: $V_0/m = 0.5$ and $m a = 5$.

Fig. 2. The phase shifts $\delta_0$ and $\delta_1$ in units of $\hbar$ as functions of the well depth $V_0$ for fixed energy: $E/m = 1.9$ and fixed width: $m a = 5$.

even and odd solutions with energy levels given, respectively, by the equations

\begin{align}
    &k_1 \tan (k_1 a) = k_0 \\
    &k_1 \cot (k_1 a) = -k_0
\end{align}

with $k_0 = \sqrt{m^2 - E^2}$. One should briefly mention that bound states do not occur if $k_1$ is imaginary since in that case Eqs. (64) and (65) have no solution. Then, when the energy of the incident wave is positive, if the potential has an even bound state close to the upper continuum (with energy $E = m$), we then have $k_1 a = \pi n$ with $n = 0$ a non negative integer, so that $c_1 = 1$ and $s_1 = 0$ and the situation 1 arises. But if this bound state is of odd parity, then we have $k_1 a = (n + 1/2)\pi$, so that $c_1 = -1$ and $s_1 = 0$, giving rise to the situation 2.

Finally, when the energy of the incident wave is negative, and if there is a bound state at the onset of the lower continuum, similar situations arise. However, unlike the case of positive energy, these situations occur only when $|V_0| > 2m$.

6. Conclusion

In summary, we have studied the relativistic quantum scattering of spinless particles in one-spatial dimension in the framework of the FV formalism as an alternative to the usual KG equation. We have constructed the general form of the scattering matrix, for symmetric and non-symmetric potentials, based on general considerations related to the properties of the FV equation. Then, we have exposed, in a pedagogical way, how a transmission-reflection problem can be described using partial-wave decomposition: in one dimension there are only two partial waves associated with even and odd parities. They are either decoupled or coupled depending on whether the scattering potential is symmetric or non-symmetric, respectively. In the non-symmetric case, the process can be described in terms of two eigenphases and a mixing parameter. As an illustration, we treated the problem of scattering by a symmetric square well potential. In particular, we discussed the behaviours of the transmission and reflection probabilities as well as the phase shifts at threshold when the momentum of the incident wave...
is close to zero. In this respect we found that such a wave can be totally transmitted if the square well potential supports a bound state at threshold.

**Declarations**

**Author contribution statement**

**Y. Chargui**: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

**A. Dhahbi, A.R. Karam**: Conceived and designed the experiments; Contributed reagents, materials, analysis tools or data; Wrote the paper.

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**Additional information**

No additional information is available for this paper.

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