Semi-Relativistic Reflection and Transmission Coefficients for Two Spinless Particles Separated by a Rectangular-Shaped Potential Barrier

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Abstract A generalized Schrödinger approximation, due to Ikhdair & Sever, of the semi-relativistic two-body problem with a rectangular barrier in (1+1) dimensions is compared with exact computations. Exact and approximate transmission and reflection coefficients are obtained in terms of local wave numbers. The approximate transmission and reflection coefficients turn out to be surprisingly accurate in an energy range |ε − V0| < 2μc2, where μ is the reduced mass, ε the scattering energy, and V0 the barrier top energy. The approximate wave numbers are less accurate.

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1 Introduction

The simplest models used for theoretical predictions of a transmission coefficient are taken from non-relativistic quantum mechanics describing a single mass particle approaching a repulsive potential barrier in one space dimension.

The non-relativistic quantum theory of relative motion of particles does not take into account two-body phenomena. It predicts the same results for any two particles with the same, common reduced mass. Two-body effects have to do with relativistic considerations; special relativity. Two-body effects may be: energy shifts of resonances and bound states, and even disappearance of exited bound states. Such relativistic effects exist for a single Dirac mass and bound states, and even disappearance of exited bound states.

The approximate wave numbers are less accurate.

The semi-relativistic quantum (SRQ) approach2–4 aims at understanding two-body effects from a simple starting point; the principles of quantum mechanics together with the energy-momentum relation of special relativity. This approach still meets mathematical problems introduced by square-root operators of the type \( \sqrt{m_j^2c^4 + p_j^2c^2} \), where \( m_j \) (\( j = 1, 2 \)) is any of the rest masses of the two particles, \( p \) being the momentum operator, and \( c \) the speed of light.

A recent analysis of the two-body barrier problem in (1+1) dimensions was treated by the so called spinless Salpeter (SSE) equation.5 This equation results from a Schrödinger-type approximation of the SRQ-equation due to Ikhdair & Sever,6 primarily for obtaining discrete energy spectra. The method has been applied to several bound-state problems7 and some of its results have been discussed and questioned by Lucha & Schöberl.8 In the present scattering context the same approximation will be referred to as the generalized Schrödinger (GS) approximation.

The present study is limited to scattering in (1+1) relativistic dimension of two spinless particle masses. Exact results for the rectangular potential model are compared to results based on the generalized Schrödinger (GS-) approximation and those of the non-relativistic Schrödinger approximation. The non-relativistic Schrödinger theory depends only on the reduced mass of the particles. Therefore, it is instructive to present two-body results with a given reduced mass.

The potential is given by

\[ V(x) = V_0, \quad -a < x < a, \quad V(x) = 0, \quad |x| \geq a. \]  \hspace{1cm} (1)

A limit for the potential strength \( V_0 \) is introduced, having to do with the physical understanding of the scattering results. The potential range \( a \) is varied, as it appears to be particularly important for the occurrence of oscillations in the transmission coefficient as function of the scattering energy.

Section 2 formulates the semi-relativistic two-body problem. Section 3 presents an analytic solution of the non-relativistic and the generalized Schrödinger problems for the potential model used. Illustrations and results are presented in Sec. 4. Conclusions are given in Sec. 5.

2 Quantum-Mechanical Two-Particle Equations with Relativistic Corrections

The total linear momentum is conserved and the centre-of-mass relative momenta are related by the classical vector equation \( \mathbf{p}_2 = -\mathbf{p}_1 \). Therefore, a single operator symbol \( \widehat{p} = -i\hbar d/dx \) is introduced, \( \hbar \) being the
reduced Planck’s constant. This operator describes the relative motion of two particles with masses \( m_1 \) and \( m_2 \) along an \( x \)-axis in a center-of-mass reference system. The SRQ-wave function \( \psi \) for the relative motion satisfies the equation:

\[
\left( \sqrt{m_1^2 c^4 + \beta^2 c^2} + \sqrt{m_2^2 c^4 + \beta^2 c^2} + V(\hat{x}) \right) \psi = M \psi,
\]

where \( M = (m_1 + m_2)c^2 + \epsilon \) is the total energy, and \( \epsilon \) is the (non-rest) scattering energy.

In regions of no interaction potential, the free wave (a plane wave \( \psi_k = e^{i\hat{x}x} \)) satisfies

\[
\hat{p}^2 \psi_k = \hbar^2 k^2 \psi_k, \quad (V = 0),
\]

where \( k \) is the “free” wave number away from the barrier. This implies, by expanding the square-root operators in Eq. (2), that

\[
\left( \sqrt{m_1^2 c^4 + k^2 \hbar^2 c^2} + \sqrt{m_2^2 c^4 + k^2 \hbar^2 c^2} \right) \psi_k = (mc^2 + \epsilon) \psi_k,
\]

where \( m = m_1 + m_2 \) is the total mass.

In the asymptotic (potential-free) regions, the relation between the wave number and the energy is

\[
\sqrt{m_1^2 c^4 + k^2 \hbar^2 c^2} + \sqrt{m_2^2 c^4 + k^2 \hbar^2 c^2} = mc^2 + \epsilon,
\]

or equivalently

\[
\left\{ \begin{aligned}
\frac{1}{m_1} &+ \frac{1}{1 + \sqrt{1 + k^2 \hbar^2 / m_1^2 c^4}} \\
\frac{1}{m_2} &+ \frac{1}{1 + \sqrt{1 + k^2 \hbar^2 / m_2^2 c^4}}
\end{aligned} \right\} \hbar^2 c^2 = \epsilon,
\]

obtained by standard algebraic manipulations.

By solving Eq. (5) (or Eq. (6)) for the asymptotic wave number, one obtains

\[
k = \frac{1}{2\hbar c} \sqrt{\frac{2mc^2 + \epsilon}{(mc^2 + \epsilon)^2}}
\]

where the variable coefficient

\[
\mu = \frac{m_1 m_2}{m_1 + m_2}.
\]

The wave numbers \( k \) and \( k_{NR} \) are positive for all \( \epsilon > 0 \).

In the barrier region of the rectangular potential (1) the wave number of a plane wave is denoted \( k_n \), and is given by

\[
k_n = \frac{1}{2\hbar c} \sqrt{(\epsilon - V_0)(2mc^2 + \epsilon - V_0)(2m_1c^2 + \epsilon - V_0)(2m_2c^2 + \epsilon - V_0)}.
\]

\[\mu\]

**Note** When considering the wave function describing the motion of both particles, say \( \psi_1 + \psi_2 \), one needs a superposition of two waves traveling in opposite directions. Then one wave function, say \( \psi_1 \), would be defined above and the other one, \( \psi_2 \), defined by space-reflected boundary conditions. In this case interference effects occur, and the phases of the amplitudes \( r \) and \( t \) become important. Such considerations are ignored in the present study.

The plane-wave solutions of the SRQ equations, and their derivatives, are fitted at the two boundary positions \( x = \pm a \) of the rectangular barrier, yielding the transmission coefficient

\[
T = \frac{1}{1 + ((k^2 - k_{NR}^2)/(4k^2 k_{NR}^2)) \sin^2(2ak_n)}
\]

and

\[
R = 1 - T,
\]

which is valid at all energies \( \epsilon > 0 \). Note in Eq. (14) that \( \sin^2 \) for energies \( \epsilon > V_0 \) turns into a sinh\(^2\)-behavior for \( \epsilon < V_0 \) (see Sec. 4 below).

### 3 Generalized Schrödinger Method

The generalized Schrödinger (GS) equation for the two-body problem is given by:[2,4-5]

\[
\frac{d^2 \psi}{dx^2} + K_{GS}^2 \psi = 0,
\]

where the variable coefficient \( K_{GS}^2 \) is

\[
K_{GS}^2 = \frac{2\mu}{\hbar^2} (\epsilon - V) + \frac{\eta_{GS}}{\hbar^2 c^2} (\epsilon - V)^2,
\]

containing a two-body mass index

\[
\eta_{GS} = \left( \frac{m_1}{m} \right)^3 + \left( \frac{m_2}{m} \right)^3 = 1 - \frac{3\mu}{m}.
\]

This index \( \eta_{GS} \) appears only in the approximate theory and having numerical values in the range \( 1/4 \leq \eta_{GS} \leq 1 \), attaining the minimum value for equal masses; see Ref. [4].
Equation (15) is equivalent to the spinless Salpeter equation (SSE) introduced by Ikhdair in Ref. [2], and in earlier references therein. It has been applied by others; to scattering transmission[5] and to bound-state spectra.[6] It can for exponential-type potentials often be treated by transforming it to a standard differential equation of the hyper-geometric type. For the rectangular barrier case such transformations are not needed. The non-relativistic problem is covered by Eq. (16), where in \( K_{GS}^2 \) and \( \kappa_B \) below in Eq. (19) one puts \( \eta_{GS} = 0 \).

The generalized Schrödinger formula for the transmission (and reflection) coefficient would be similar to Eq. (14), but with different wave numbers. For notational simplicity the approximate wave numbers are denoted by \( \kappa \) (instead of e.g. \( k_{GS} \)). Hence, the off-barrier GS-wave number is

\[
\kappa = \sqrt{\frac{2\mu}{\hbar^2}} \xi + \frac{\eta_{GS}}{\hbar^2 c^2} \xi^2 \tag{18}
\]

while in the barrier region one has

\[
\kappa_B = \sqrt{\frac{2\mu}{\hbar^2}} (\epsilon - V_0) + \frac{\eta_{GS}}{\hbar^2 c^2} (\epsilon - V_0) \tag{19}
\]

The approximate transmission coefficient is given by

\[
T_{GS} = \frac{1}{1 + \left[ (\kappa^2 - \kappa_B^2)^2 / 4\kappa^2 \kappa_B^2 \right] \sin^2(2\kappa_B a)} , \tag{20}
\]

and \( R = 1 - T \). (GS)

The non-relativistic transition coefficient would be obtained from Eqs. (19) and (20) with \( \eta_{GS} = 0 \). The non-relativistic transition coefficient does not show two-body effects and is not illustrated in the subsequent section.

4 Results and Illustrations

Results are presented in units such that \( c = \hbar = m_u = 1 \), where \( m_u \) is a mass unit. The length unit \( (x_u = 1) \) corresponds to the Compton wave length \( (h/(m_u c^2)) \). The individual particle masses are denoted \( m_1 \) and \( m_2 \) in such mass units. One of the masses, \( m_2 \), is determined in this study by \( m_1 \) and the reduced mass \( \mu \). This choice of keeping the reduced mass as a primary mass parameter is motivated by the fact that non-relativistic results only depend on the reduced mass. The mass \( m_1 \) is chosen to be the “large” mass so that \( m_1 \geq 2\mu \).

The two-body effects in this study have to do with the different mass combinations for the same reduced mass \( \mu \). Equal masses are represented by \( m_1 = 2\mu \) in the computations, and unequal masses are represented by \( m_1 = 100\mu \).

Transmission and reflection coefficients depend on the wave numbers in and off the barrier region. It is relevant to understand the approximate and exact wave numbers before a comparison of the transmission coefficients.

4.1 Wave Numbers

The wave numbers \( k_B \) and \( \kappa_B \) seem analytically different. With the restricted condition \( V_0 < 2m_2 c^2 \), a numerical investigation of their squares shows that the approximate wave number \( \kappa_B^2 \) is a reasonably good approximation of \( k_B^2 \) in a large range of realistic potential parameters.
A potential barrier with $V_0 = 1\mu$ and $\mu$ of the order of the relativistic mass unit ($m_u = 1$) shows good agreement between $\kappa^2_B$ and $k^2_0$. Their difference is plotted in Fig. 1, against $\epsilon/V_0$. Dashed curves in Fig. 1 represent equal masses and solid curves represent unequal masses for the same reduced mass. Red curves represent non-relativistic wave numbers, obtained by putting $\eta = \kappa_B = 0$ in the GS formulas.

Errors in the GS barrier wave numbers increase significantly for unequal masses and $V_0$ (or $\mu$) increasing beyond the unit mass. The GS approximation seems to be excellent for the equal-mass case (blue, dashed curves). The non-relativistic approximation is only valid for scattering energies close to the barrier top energy.

For the same barriers as in Fig. 1, the off-barrier wave numbers are studied in Fig. 2. The non-relativistic (red curves) are accurate only near $\epsilon \approx 0$ unless the reduced mass is much smaller than the relativistic mass unit. The GS-approximation improves the non-relativistic off-barrier wave numbers significantly, although not as much as it improves the barrier wave numbers. The equal-mass cases (blue, dashed curves) in Fig. 2 show no errors in the GS approximation.

![Fig. 2 Approximation error in $\kappa^2$ (blue curves) as function of $\epsilon/V_0$ for $V_0 = \mu$ with $\mu = 5, 2, 1,$ and 0.5 mass units. Solid lines represent unequal masses with $m_1 = 10\mu$ and dashed lines represent equal masses where $m_1 = 2\mu$. Red lines, tending to negative values as $\epsilon$ increases, correspond to errors of the non-relativistic wave numbers for which $\eta = 0$ in the GS formulas.](image)

### 4.2 Transmission Coefficient

Because of the relation between the transmission and reflection coefficients, $T + R = 1$, it is sufficient to analyze just the transmission coefficient $T$. The formulas (14) and (20) indicate that the wave numbers play an important role. The over-barrier case of scattering energies allow oscillations depending on the barrier wave numbers and the barrier size $a$. The off-barrier wave numbers affect the magnitudes of the amplitudes of the oscillations only, not the frequencies of the oscillations. For wide barriers, small errors in the barrier wave numbers may still be significant for the oscillation phases at energies $\epsilon \gg V_0$.

The error in the oscillation pre-factor $(\kappa^2 - \kappa_0^2)/(4\kappa^2\kappa_0^2)$ is more difficult to understand. In Fig. 3 the absolute error is denoted

$$\Delta \gamma = |(\kappa^2 - \kappa_0^2)/(4\kappa^2\kappa_0^2) - (k^2 - k_0^2)/(4k^2k_0^2)|.$$  

(21)

The parameters and energies used in Fig. 3 are those taken as those in Figs. 1 and 2. The error $\Delta \gamma$ for the case of unequal masses (solid curves) changes sign and seems to be almost independent of potential and mass parameters, despite the significant differences due to parameters of the wave numbers in Figs. 1 and 2. This error is singular in a transition region where the scattering energy is near the barrier top energy, and also close to the threshold limit $\epsilon = 0$. Well inside the over-barrier and the under-barrier energy regions the errors are small. The singularities are cancelled by the fact that $\kappa$ agrees with $k$ as $\epsilon \rightarrow 0$, and $\kappa^2_0$ agrees with $k^2_0$ as $\epsilon \rightarrow V_0$. In the barrier transition region there is a sign change in $\kappa^2_0$ and in the oscillation pre-factor $(\kappa^2 - \kappa_0^2)/(4\kappa^2\kappa_0^2)$. In the same region one has

$$\sin^2(2\kappa_0 a) \approx 4\kappa_0^2 \kappa^2_0, \quad |\kappa_0| \approx 0,$$  

(22)

which cancels $\kappa^2_B$ in the pre-factor and the over-all sign change. As a result of the apparent independence of $\Delta \gamma$ as potential parameters are changed, the main source of error in the transmission coefficient seems to be the argument of the sine function, $4\kappa_0 B$, when this is real valued (over-barrier case). The spatial range of the potential magnifies the positive error in $\kappa_B$ for $a > 1$. The GS approximation
predicts shorter energy periods of the possible oscillations in $T$, as $\epsilon(> V_0)$ increases. For scattering energies below $V_0$, $T$ is non-oscillatory and usually vanishing as $\epsilon \to 0$. The sine function has turned exponentially increasing as $\epsilon$ approaches zero, while $V_0$ being not too small. Errors in $T$ are then less likely to be observed for the parameters used in Figs. 1–3.

Fig. 3 Absolute GS-approximation error, $\Delta \gamma$, in the oscillation pre-factor (Eq. (21)) as function of $\epsilon/V_0$ with $V_0 = \mu$ and $\mu = 5, 2, 1,$ and 0.5 mass units. The equal mass case (dashed line) does not show any significant numerical error.

Fig. 4 Transmission coefficients for a barrier range $a = 1$, and other parameters being as in Figs. 1–3. The equal mass cases are represented by dashed curves and the unequal mass cases represented by solid curves. Figure 4 shows the transmission coefficient for a barrier range $a = 1$ and for other parameters as in Figs. 1–3. Two-body effects are significant in all four subplots of Fig. 4, although not for $\epsilon \approx V_0$. The GS-approximation results (surprisingly) agree with those of exact calculations (see Table 1), and results are represented by common curves. The dashed curves ($m_1 = 2\mu$) and solid curves ($m_1 = 100\mu$) differ slightly in their wavy behaviors. This is the two-body effect seen in Fig. 4, which is well predicted by the GS-approximation.

Figure 5 considers a three times wider barrier with $a = 3$. Again, the results of the GS-approximation are in-
distinguishable from the exact results on the scale of the figures. The two-body effects here, predictable by the GS-approximation, appear as shifts of transmission peaks for over-barrier energies. These shifts gradually increase as the energy increases.

Table 1 shows numerical results for the transmission coefficient related to Fig. 5 for $\mu = 5$, and selected values of the scattering energy. In this table results are compared with those of the GS-approximation. In the equal-mass case ($m_1 = 2\mu$) in Table 1 both entries are identical. It can be confirmed (not included in the present work) that the transmission coefficients $T$ and $T_{GS}$ are analytically the same in the equal-mass case. For “light-heavy” masses the differences between $T$ and $T_{GS}$ are still small on the graphical scales in Figs. 4 and 5.

The table, as well as Figs. 4 and 5, show significant two-body effects for all system parameters, unless the transmission coefficient is exponentially small.

Fig. 5 Transmission coefficients for a barrier range $a = 3$ and other parameters are as in Figs. 1–3. The equal mass cases are represented by dashed curves and the unequal mass cases represented by solid curves.

Table 1 Two-body transmission coefficients $T$ and $T_{GS}$ are compared for selected scattering energies ($\epsilon/V_0$). The potential parameters are $V_0 = 1\mu$ and $a = 3$, and the results correspond to Fig. 5, for $\mu = 5$.

<table>
<thead>
<tr>
<th>$\epsilon/V_0$</th>
<th>$m_1/\mu$</th>
<th>$T_{GS}$</th>
<th>$T$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8</td>
<td>100</td>
<td>$4.2 \times 10^{-16}$</td>
<td>$4.2 \times 10^{-16}$</td>
</tr>
<tr>
<td>0.8</td>
<td>2</td>
<td>$1.3 \times 10^{-16}$</td>
<td>$1.3 \times 10^{-16}$</td>
</tr>
<tr>
<td>1.2</td>
<td>100</td>
<td>0.447 69</td>
<td>0.449 48</td>
</tr>
<tr>
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<td>2</td>
<td>0.868 61</td>
<td>0.868 61</td>
</tr>
<tr>
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<td>100</td>
<td>0.943 83</td>
<td>0.937 28</td>
</tr>
<tr>
<td>1.6</td>
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<td>0.933 64</td>
<td>0.933 64</td>
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<tr>
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<td>0.598 20</td>
<td>0.599 83</td>
</tr>
<tr>
<td>2.0</td>
<td>2</td>
<td>0.891 52</td>
<td>0.891 52</td>
</tr>
</tbody>
</table>

5 Conclusions

The rectangular potential allows exact numerical semi-relativistic calculations, involving linear plane waves only and their matching at the barrier discontinuities. The generalized Schrödinger (GS) approximation seems to predict accurate energy behavior of the transmission coefficient in a reasonably realistic energy range. With the scales of the illustrations, the GS results are indistinguishable from those of the exact computations of the transmission coefficient and significant two-body effects are accurately obtained.

Two-body effects in the present illustrations appear mainly as energy shifts of total transmission in the over-barrier energy region. These effects may seem more striking in numerical tables, like in Table 1, where in the over-barrier case oscillations may be dense on the energy scale and of quite large amplitudes; see Figs. 4–5. In the under-barrier case two-body effects appear stronger for smaller values of the reduced mass (compare Figs. 4 and 5).

The observed accuracy of the GS approximation does
not apply to the local wave numbers, but errors appear to cancel in the final formula for the transmission coefficient. In a more rigorous study on two-body interference effects, discussed in the final paragraphs of Sec. 2, this situation may no longer prevail if the barrier energy $V_0$ is of the order of $m_2c^2$ or much larger.

References


