Isospectral scattering for relativistic equivalent Hamiltonians on a coarse momentum grid

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The scattering phase-shifts are invariant under unitary transformations of the Hamiltonian. However, the numerical solution of the scattering problem that requires to discretize the continuum violates this phase-shift invariance among unitarily equivalent Hamiltonians. We extend a newly found prescription for the calculation of phase shifts which relies only on the eigenvalues of a relativistic Hamiltonian and its corresponding Chebyshev invariance among unitarily equivalent Hamiltonians. We illustrate this procedure numerically considering \( \pi\pi \), \( \pi N \) and \( NN \) elastic interactions which turns out to be competitive even for small number of grid points.

I. INTRODUCTION

Hadronic reactions at intermediate energies provide a working and phenomenological scheme to access to the corresponding dynamical interactions from scattering experiments and their corresponding partial wave analysis in terms of phase-shifts. Even in the simplest cases the conditions of relativity and unitarity are mandatory requirements, while the description of bound states and resonances requires a non-perturbative approach. Within a Lagrangian and covariant field theoretical setup all these demands are best encapsulated within the Bethe-Salpeter equation (BSE) [1] (see Ref. [2] for an early review), where the interaction is defined by a two-particle irreducible four-point function. In practice, this object needs to be truncated, depends on the renormalization scale and is itself off-shell ambiguous as there is a reparameterization freedom in the definition of the fields [3, 4] (see e.g. [5] for an explicit discussion of low energy interactions). The BSE is an integral 4D equation and hence presents not only many practical but also challenging conceptual mathematical challenges because scattering is naturally formulated in Minkowsky space and truncated exchange interactions display an intricate singularity structure [6] so that a full solution has only been found recently [7,8].

Due to all these complications the conventional approach to the two body relativistic problem has been the study of judicious 3D reductions of the BSE closer in spirit to the Lippmann-Schwinger equation [9] in the non relativistic case (see e.g. [10, 11] for elementary discussions), but preserving the unitarity character of the scattering amplitude. This viewpoint leads to Quasioptical or Quasipotential models proposed long ago [12]. Among the many different proposals and variants based on this idea it is worth mentioning the Blankenbecler-Sugar equation [13], the Kadyshevsky equation [14] and the Gross spectator equation [15, 16]. While any of these schemes has its advantages and disadvantages, our main results and formulas, however, can be easily extended to these other schemes with minor modifications.

In this paper we will choose for definiteness the Kadyshevsky equation [14] which befits a Hamiltonian formulation in quantum field theory. The usefulness of the Hamiltonian approach, besides providing a compelling physical picture, relies on the explicit use of a Hilbert space and becomes more evident when dealing with the few-body problem, where one expects to determine binding energies of multihadron systems in terms of their mutual interactions. Unfortunately, only in few cases, such as e.g. separable potentials, can one provide an analytical or semi-analytical solution of the relativistic two-body scattering problem and in this case one employs a numerical inversion method which implies a discretization procedure on a given momentum grid [17]. From a physical point of view, the introduction of a momentum grid corresponds to add an external interaction or to introduce a restriction on the Hilbert which constraints the energy levels of the system. A well known example corresponds to impose boundary conditions at a spherical box with finite volume and radius \( R \) which provides an equidistant momentum grid for large box sizes, \( p_n \sim \pi n / R \) [18] or equidistant energies [19]. Another example which will be relevant in this paper corresponds to diagonalizing in a Laguerre basis [20] which yields a Gauss-Chebyshev momentum grid (See [21] for a comprehensive and self-contained exposition on Chebyshev methods.). This so-called \( L^2 \)-methods [22] have clear computational advantages, but quite generally, basic properties of scattering such as the the intertwining property of the Moller wave operators does not hold [23] and is only recovered in the continuum limit.

One important aspect within the Hamiltonian approach and relevant to the present study is the notion of equivalent potentials [24, 25], i.e. the fact that unitarily equivalent Hamiltonians produce identical phase-shifts, hence they are referred to as phase-equivalent potentials. Because the eigenvalues of the Hamiltonian \( H \) are invariant under \( H \rightarrow UHU^\dagger \) with \( UU^\dagger = U^\dagger U = 1 \) we will also talk about isospectral phase-shifts, namely those that fulfill

\[
\delta_{l,H}(p) = \delta_{l,UHU^\dagger}(p)
\]
where \( l \) is the angular momentum, \( p \) the CM momentum, \( H \) is the Hamiltonian and \( U \) an arbitrary unitary transformation. On a broader context, this is the counterpart of the Lagrangian field reparameterization of the BSE [3–5]. A characterization for equivalent relativistic Hamiltonians has been proposed in Ref. [26]. It is perhaps not so well-known that the numerical methods employed to invert the scattering matrix equation generally violate this unitary equivalence, namely a unitary transformation of the Hamiltonian on the grid does not yield the same phase-shift, see Eq. (1). The effect disappears when the grid is sufficiently fine or equivalently when the number of grid points becomes large. This violation has been illustrated explicitly in the non-relativistic case [27, 28] and will also be shown to occur in the present work.

The question is that while one expects that with a fine grid the continuum limit will eventually and effectively be recovered and hence the isospectral invariance of the phase-shifts, spectral methods based on the eigenvalues provide themselves a natural and invariant definition of the phase-shift. These methods based on the Fredholm determinant originally proposed by DeWitt [19] (see also [18]) and improved by others [22] (see e.g. [29] for a review and references therein). However, while these methods are by construction isospectral for any number of grid points they are not necessarily accurate. In a recent letter [30] we have provided a method which is both isospectral and accurate for a coarse grids in the non-relativistic case. In this paper we analyze the consequences of such a method for the relativistic situation and illustrate it with several low energy, \( S, P \) and \( D \) phases for \( \pi \pi \), \( \pi N \) and \( NN \).

The present paper is organized as follows. We will review this issue and use for definiteness the Kadyshevsky equation in Section V and we review some of its properties including a proof of isospectrality. The solution of the scattering equations requires a momentum grid which may be implemented with the Gauss-Chebyshev quadrature in three different ways. In section IV we analyze three isospectral definitions of the scattering phase shifts based on the energy-shift, the momentum shift and the Chebyshev angle shift which specifically depend on the mass of the particles. In Section V we present our numerical results for some separable \( \pi \pi \), \( \pi N \) and \( NN \) model interactions. Finally, in Section VI we come to the conclusions and provide some outlook for future work.

II. RELATIVISTIC SCATTERING: THE KADYSHEVSKY APPROACH

A. Generalities

In this section we review some relevant quantities for completeness and in order to fix our notation and conventions. Elementary discussions may be found in textbooks [10, 11]. The Kadyshevsky equation in the CM frame with \( \sqrt{s} \) CM energy and in the equal mass case reads [13, 1]

\[
T(p', \bar{p}, \sqrt{s}) = V(p', \bar{p}) + \int \frac{d^3q}{(2\pi)^3} \frac{V(q, \bar{p})}{\sqrt{s} - E_q + i\epsilon} T(q, p, \sqrt{s})
\]

(2)

where the potential is symmetric \( V(p', \bar{p}) = V(\bar{p}, p') \) and energy independent. These two conditions are necessary in order to check unitarity, since

\[
T(p', \bar{p}, \sqrt{s}) - T(p, \bar{p}, \sqrt{s}) = \int \frac{d^3q}{(2\pi)^3} \frac{2\pi i\delta(\sqrt{s} - 2E_q)}{4E_q^2} \times \frac{T(q, \bar{p}, \sqrt{s})T(q, p, \sqrt{s})^*}{E_q^2} \tag{3}
\]

A residual ambiguity of the Kadyshevsky equation has been discussed in Ref. [31] and the 3D-reduction of the BS equation with a separable kernel has been addressed [32]. The 3D-reduction of the relativistic three-body Faddeev equation associated to the this quasipotential was proposed afterwards [33]. As compared to other approaches [34], this particular 3-D reduction satisfies a Mandelstam representation, i.e. a double dispersion relation both in the invariant mass \( s \) and momentum \( t \) Mandelstam variables [35]. The appearance of spurious singularities has been addressed in the different approaches in Ref. [36]. In addition, the Kadyshevsky equation also lacks spurious singularities in the related three-body problem [37]. Actually, there has been already some work with this equation for the case of \( \pi \pi \), \( NN \) and \( NN \) scattering [38] for separable potentials where the lowest partial waves corresponding to \( S, P \) and \( D \) angular momenta have been fitted which will be discussed below in more detail.

B. Partial waves

This 3D scheme has the advantage that besides enabling a relativistic Hamiltonian interpretation for the scattering problem they also become amenable to numerical analysis since at the partial waves level they reduce to 1D linear integral equations. Using rotational invariance

\[
T(p', \bar{p}, \sqrt{s}) = 4\pi \sum_{lm} Y_m(p') Y_l(\bar{p})^* T_l(p', p, \sqrt{s}) \tag{4}
\]

At the partial waves level and for spin zero equal mass particles we get

\[
T_l(p', p, \sqrt{s}) = V_l(p', p) + \int_0^\infty dq \frac{q^2}{4E_q^2} \frac{V_l(p', q)T_l(q, p, \sqrt{s})}{\sqrt{s} - 2E_q + i\epsilon} \tag{5}
\]

1 The case of two different masses corresponds to replace \( E_q^2 \rightarrow E_q \alpha_q \) and \( \sqrt{s} = 2E_q \rightarrow E_q + \alpha_q \) with \( E_q = \sqrt{m^2 + q^2} \) and \( \alpha_q = \sqrt{m^2 - q^2} \). We will keep the equal mass case because the formulas are much simpler for presentation purposes and will return to this situation when analyzing the \( \pi N \) case.

2 We restrict ourselves to central isotropic interactions. The important case of tensor anisotropic potentials leading to coupled channels presents some differences and complications and will be discussed in a separate publication.
where \( +ie \) implements the original Feynman boundary condition of the BSE and corresponds to outgoing spherical waves, \( E_q = \sqrt{q^2 + m^2} \) and on the mass shell one has \( \sqrt{s} = 2\sqrt{p^2 + m^2} \) with \( p \) the CM momentum. For a real potential this equation satisfies the two-body unitarity condition, so that the phase-shift is given by

\[
T_i^{-1}(p, p, \sqrt{s}) = -\frac{\pi p}{8E_p} \{ \cot \delta_i(p) - i \} .
\]

Alternatively we may define the reaction matrix \( R_l \)

\[
T_i^{-1}(p, p, \sqrt{s}) = R_l^{-1}(p, p, \sqrt{s}) + i\frac{\pi p}{8E_p} ,
\]

so that

\[
-\tan \delta_i(p) = \frac{\pi p}{8E_p} R_l(p, p, \sqrt{s}) ,
\]

where the corresponding reaction matrix satisfies the equation

\[
R_l(p', p, \sqrt{s}) = V_i(p', p) + \int_0^\infty dq \frac{q^2}{4E_q^2} V_l(q, p) R_l(q, p, \sqrt{s}) ,
\]

where the principal value has been integrated in the integral. As it is well known we can implement the principal value by means of a subtraction using the trivial identity

\[
\int_0^\infty \frac{2k_0 dp}{p^2 - k_0^2} = \int_{-\infty}^\infty \frac{dp}{p - k_0} = 0 ,
\]

whence follows the integration rule

\[
\int_0^\infty dp \frac{f(p)}{2E_0 - 2E_k} = \int_0^\infty dp \left[ \frac{f(p)}{2E_0 - 2E_k} - \frac{f(k_0)E_0}{k_0^2 - p^2} \right] ,
\]

where \( \sqrt{s} = 2E_0 = \sqrt{k_0^2 + m^2} \). Using this we get

\[
R_l(p', p, \sqrt{s}) = V_i(p', p) + \int_0^\infty dq \left[ \frac{q^2}{4E_q^2} V_l(q, p) R_l(q, p, 2E_0) - \frac{k_0^2}{k_0^2 - q^2} V_l(q, k_0) R_l(k_0, p, 2E_0) \right] .
\]

In the continuum the Eqs. (5), (9) and (12) are fully equivalent, but discretized versions provide different results, all of them violating the isospectrality of the phase-shifts, as will be shown in Section III C.

Note that for our normalization convention in the spherical basis we have the closure relation

\[
1 = \int_0^\infty dq \frac{q^2}{4E_q^2} \langle q | q \rangle .
\]

As it is well known, bound states appear as poles of the scattering matrix. This allows to define a Hamiltonian in the CM system,

\[
H \Psi_i(p) = 2E_p \Psi(p) + \int_0^\infty dq \frac{q^2}{4E_q^2} V_l(q, p) \Psi_i(q) ,
\]

so that the homogeneous Kadyshevsky equation reads

\[
H \Psi_i(p) = \sqrt{s} \Psi_i(p) .
\]

While this equation is usually meant to solve for the bound state problem, we will actually show below how it can also be used to solve the scattering problem on a finite momentum grid.

### C. Scattering equivalence

One of the most remarkable features of quantum scattering is the lack of uniqueness of the interaction; under unitary transformations of the Hamiltonian the S-matrix, or equivalently the phase-shifts remain invariant. In this section we remind of this fact by considering the continuum limit first. We will then see that its discretized counterpart through a finite momentum grid does not preserve this symmetry if the corresponding phase-shifts are defined as in Eq. (14).

In operator form \( V(p', \bar{p}) \equiv \langle \bar{p} | V | p \rangle \) and \( T(p', \bar{p}, \sqrt{s}) \equiv \langle \bar{p} | T(\sqrt{s}) | p \rangle \) and the Kadyshevsky equation written as a Lippmann-Schwinger reads

\[
T = V + VG_0T = V + GV
\]

\[
= V(1 - G_0V)^{-1} = (1 - VG_0)^{-1} V
\]

which we write alternatively in equivalent forms and have defined \( G^{-1} = \sqrt{s} + ie - H = G_0^{-1} - V \). Within this Hamiltonian framework, in the continuum, we consider a unitary transformation \( U \) of the Hamiltonian \( H \), given by \( H \rightarrow \bar{H} = UHU^\dagger = H_0 + V \) where \( V = UHU^\dagger - H_0 \). Taking the exponential representation of a unitary operator \( U = e^{i\xi} \) with \( \xi = \xi^\dagger \) a self-adjoint operator, for an infinitesimal transformation we have lowest order \( U = 1 + i\xi + \mathcal{O}(\xi^2) \) and hence \( \Delta V = i[\xi, H] \). If we take the form \( T^{-1} = V^{-1} - G_0 \) we have, \( \Delta V^{-1} = -V^{-1}\Delta VV^{-1} \) and similarly for \( T \) so that

\[
\Delta T = TV^{-1}\Delta VV^{-1}T
\]

\[
= (1 - G_0V)^{-1} \Delta V(1 - VG_0)^{-1}
\]

\[
= G^{-1}_0 G[\xi, H] G G_0^{-1}
\]

\[
= (1 + TG_0) \xi G_0^{-1} - G_0^{-1} \xi (1 + G_0T)
\]

where we have used the Eqs. (18). Thus, taking matrix elements and because of the external factors \( G_0^{-1} \) we get in the limit \( e \rightarrow 0 \) at the on shell point \( 2E_p = 2E'_p = \sqrt{s} \) the result

\[
\Delta T(p', \bar{p}) \bigg|_{2E_p = 2E'_p = \sqrt{s}} = 0
\]

Thus, for a given generator \( \xi = \xi^+ \) we have that

\[
\Delta V = i[\xi, H] \implies \Delta \delta_i(p) = 0 .
\]

or equivalently, for finite transformations \( \delta_iH(p) = \delta_iUHU^\dagger(p) \).
III. DISCRETIZATION SCHEMES AND SCATTERING INEQUIVALENCE

A. Momentum grid

There are only few cases where the scattering equations can be solved analytically. The momentum grid discretization introduces both an infrared $\Delta p$ as well as an ultraviolet numerical cut-off, $\Lambda_{\text{num}}$. In our previous work we used a Gauss-Chebyshev grid [30] for interactions which have a fast fall-off. However, the kind of hadronic interactions we will be dealing with here to illustrate our method have long tails in momentum. Thus, we consider a Gauss-Chebyshev quadrature which is re-scaled in such a way that we distinguish two sub-divisions within the $[0, \infty)$ integration range. Namely, half of the grid points are arranged within interval $[0, \Lambda_{1/2}]$, and the other half are distributed along the $[\Lambda_{1/2}, \infty)$. The parameter $\Lambda_{1/2}$ is chosen in order to select the region of interest. In this way, the long-tails effects are broadly taken into account and at the same time the physical region of interest is covered with an enough density of points. This allows us to study the region of interest in detail, without neglecting long-tails effects. The grid differs then from the Gauss-Chebyshev parametrization used in our non-relativistic $NN$-scattering study [30], and is given by

$$p_n = \frac{1 + z_n}{1 - z_n}, \quad w_n = \frac{2\Lambda_{1/2}}{(1 - z_n)^3}dz_n,$$

with

$$z_n = \cos \left[ \frac{\pi}{N} \left( n - \frac{1}{2} \right) \right],$$

$$dz_n = \frac{\pi}{N} \sin \left[ \frac{\pi}{N} \left( n - \frac{1}{2} \right) \right].$$

where $n = 1, \ldots, N$. The parameter $\Lambda_{1/2}$ selects the interval $[0, \Lambda_{1/2}]$ that contains the first $N/2$ points. The lowest and highest momenta in the grid are

$$p_{\text{min}} = p_1 = \frac{1 - \cos \left( \frac{\pi}{2N} \right)}{1 + \cos \left( \frac{\pi}{2N} \right)},$$

$$p_{\text{max}} = p_N = \frac{1 - \cos \left( \frac{\pi}{2} \right)}{1 + \cos \left( \frac{\pi}{2} \right)}.$$

For a large grid and for $n \ll N$ we have $p_n = \Lambda (\pi n / 2N)^2 / 2$ which differs from the spherical box quantization. The integration rule becomes

$$\int_0^p dp f(p) \to \sum_{n=1}^N w_n f(p_n).$$

On the momentum grid, the Hamiltonian is defined as

$$H \Psi_n = 2E_n \Psi_n + \sum_k w_k \frac{p_k^2}{4E_k^2} V_{nk} \Psi_k$$

where $\Psi_n \equiv \langle p_n | \Psi \rangle = \Psi(p_n)$ and $V_{nk} = V(p_n, p_k)$. The closure relation on the grid is given by

$$\sum_n |p_n\rangle \frac{w_n p_n^2}{4E_n^2} \langle p_n| = 1.$$}

While these factors are ubiquitous, they are a bit annoying because the hermiticity does not correspond to invariance under interchange of files and rows. Therefore we define the barred basis

$$|p_n\rangle = \frac{\sqrt{w_n} p_n}{2E_n} |\overline{p_n}\rangle$$

so that the barred Hamiltonian reads

$$\overline{H}_{nk} = \left( \frac{\sqrt{w_n} p_n}{2E_n} \right) - 1 H_{nk} \frac{\sqrt{w_k} p_k}{2E_k} = 2E_k \delta_{nk} + \nabla_{nk}$$

which are obviously Hermitean, $\overline{H}_{nk} = \overline{H}_{kn}$ and $\nabla_{nk} = \nabla_{kn}$. Within this so that an infinitesimal unitary transformation generates a change $\Delta V = i[\xi, H]$ on the grid, which in the partial waves barred basis reads

$$\Delta \nabla_{nk} = -\Delta \nabla_{kn} = i \sum_{l=1}^N [\xi_l H_{ln} - \overline{H}_{kl} \xi_l]$$

where we have dropped the angular momentum $l$ for simplicity. We can then proceed to discuss the discretization of Eqs. [9], [12] which basically fall into two categories: schemes where just the grid points are needed and schemes where additional observation points are added.

It is worth noticing that unlike standard solution methods, where the energy, $\sqrt{s}$, and momentum, $p$, grids are independent from each other (see e.g. [10]), here we will address versions of the scattering equation which invoke only momentum grid points. However, as it was shown in [28, 39] for the non-relativistic case, this definition of the phase-shift is not invariant under unitary transformations on the finite momentum grid. The phase inequivalence goes away in the continuum limit $\Delta p \to 0$ corresponding to $N \to \infty$. It must also be said that the numerical problem can be also formulated following the Haftel-Tabakin procedure [17], which provides a value of the reaction matrix at any point outside the momentum grid (the so-called observation point). However, in order to consider a family of scattering-equivalent Hamiltonians, which are known in a given momentum grid, the calculation of matrix elements at points outside the grid, would require some extrapolation.
B. Scattering amplitude on the grid

In order to illustrate the lack of isospectrality in the finite momentum grid, let us consider the discretized version of the equation Eq. (5) with a finite \( \varepsilon \) and an arbitrary energy \( e = \sqrt{s} = 2 \sqrt{p^2 + m^2} \). This corresponds to take matrix elements of the operator form, so that

\[
T_{nm}(\sqrt{s}) = V_{nm} + \sum_{k=1}^{N} \frac{w_k p_k^2}{4E_k^2} \left( \frac{1}{\sqrt{s} - 2E_k + ie} \right) V_{nk} T_{km}(\sqrt{s})
\]

which in the barred basis becomes

\[
\mathcal{T}_{nm}(\sqrt{s}) = \mathcal{V}_{nm} + \sum_{k=1}^{N} \frac{\mathcal{V}_{nk} \mathcal{T}_{km}(\sqrt{s})}{\sqrt{s} - 2E_k + ie}
\]

Let us remind that the meaning of this equation is to take the continuum limit before the limit \( \varepsilon \rightarrow 0 \). In practice, this corresponds to assume \( w_n/\varepsilon \ll 1 \) and a practical consequence is the strict loss of unitarity since the delta function on the grid becomes smears as a Lorentz function. Nonetheless, we may take the prescription (K1)

\[
\text{Re}[T^{-1}_t(2E_n)]_{nn} = -\frac{\pi p_n}{8E_n} \cot \xi_k(p_n)
\]

which corresponds to the real part of Eq. (6) on the grid. In any case, under a unitary finite dimensional transformation the chain of relations leading to Eq. (19) follow, and thus in the momentum grid we have (for finite \( \varepsilon \) and unrestricted summation)

\[
\Delta T_{nm}(2E_n) = \sum_{m=1}^{N} \frac{4(E_n - E_m)\varepsilon}{3(E_n - E_m)^2 + \varepsilon^2} \mathcal{V}_{nm} \mathcal{T}_{nm}(2E_n)
\]

which is non-vanishing, unless the continuum limit is taken. Although the solution based on this method is not terribly accurate it serves the purpose of illustrate our point. We have also numerically checked that for particular unitary transformations \( U \) inducing the change \( V \rightarrow \tilde{V} \equiv U H U^\dagger - H_0 \) the phases from the Eq. (37) are indeed not invariant, unless a large number of grid points is considered.

C. Reaction matrix on the grid

The scattering problem for the reaction matrix associated with the Kadyshevsky equation for the half-off shell reaction matrix on the grid reads (the limit \( \varepsilon \rightarrow 0 \) is already taken)

\[
R_{nm} = V_{nm} + \sum_{k=1}^{N} V_{nk} w_k \frac{p_k^2}{4E_k^2} \frac{1}{2E_m - 2E_k} R_{km}
\]

where \( R_{nm} \equiv r(p_n, p_m, 2E_m) \) and the restricted sum, \( \sum_{k, s} \), implements in the momentum grid the principal value prescription. This problem can directly be solved by \( N \) matrix inversions for every single energy \( E_n \) in the grid, whence the phase-shift can be extracted using Eq. (8) evaluated on the grid points (prescription K2),

\[
-\tan \delta^{K2}_k(p_n) = \frac{\pi p_n}{8E_n} R_{nm}
\]

D. Scattering on the grid with observation points

Finally, let us consider the original approach of Haftel and Tabakin for Eq. (12), where in addition to the grid points, \( p_1, \ldots, p_N \), the notion of observation point, say \( k_0 \neq p_n \), is introduced. The algorithm to find the phases is given by the equation

\[
R(p, k_0, 2E_0) = V(p, k_0) + \sum_{k=1}^{N} \frac{w_k p_k^2}{4E_k^2} V(p, p_k) R(p_k, k_0, 2E_0)
\]

where \( E_k = \sqrt{p_k^2 + m^2} \) and \( E_0 = \sqrt{k_0^2 + m^2} \). Taking \( p = p_n \) and \( p = k_0 \) one generates \( N+1 \) equations. To ease the notation we define \( \rho_{n0} = R(p_n, k_0, 2E_0) \) and \( \rho_{00} = R(k_0, k_0, 2E_0) \), so that the equations read

\[
\rho_{n0} = V_{n0} + \sum_{k=1}^{N} D_k V_{nk} \rho_{k0} + D_0 V_{n0} \rho_{00}
\]

\[
\rho_{00} = V_{00} + \sum_{k=1}^{N} D_k V_{0k} \rho_{k0} + D_0 V_{00} \rho_{00}
\]
which is non-vanishing. Non-perturbatively we may take spe-
whether the observation point is included or not in the unitary 

Here we will present three different alternatives 

where

In the continuum $D_0$ vanishes, but on the finite grid it actually 

The question if we can check whether the calculated phase-
shift, or $\rho_{00} = R(k_0, k_0, 2E_0)$, at the observation point $k_0$ is 

so that because in any case $\Delta V_{00} = 0$ and 

where $H_{0l} = V_{0l}$ and $H_{lk} = 2E_l \delta_{lk} + V_{lk}$ and we have 

which is non-vanishing. Non-perturbatively we may take spe-
cific unitary transformations. While the observation points can 

IV. ISOSPECTRAL PHASE-SHIFTS

The requirement of isospectrality naturally suggests to deter-
determine the phase shifts from the spectrum of the Hamiltonian,
a fact noted by DeWitt [19] and Fukuda and Newton [18] 

long ago based on equidistant energy or momentum grids re-
spectively. Here we will present three different alternatives 

be analyzed in the next section. On the momentum grid, the 
eigenvalues equation can be written as

where $\Psi_n \equiv \langle p_n | \Psi \rangle$. Denoting the $N$ eigenvalues and eigen-
functions as

we write the energy in the form

This prescription is a consequence of describing the scattering 
problem in a box and imposing the physical condition of a 
vanishing wave function in the wall (see [30] for a reexamina-
tion). It is equivalent to a trapezoidal rule quadrature, and for a 
Chebyshev grid can be written as

where $\rho_{ln}$ is the “distorted” momentum by the interaction. As 
it was proposed in [18] and exemplified in [28, 39] the phase-
shift can be identified as the momentum shift in units of the 
momentum resolution, namely

\[
\delta_n(p_n) = -\pi \frac{p_n - p_n}{\Delta p_n}.
\]

This prescription is a consequence of describing the scattering 
problem in a box and imposing the physical condition of a 
vanishing wave function in the wall (see [30] for a reexamina-
tion). It is equivalent to a trapezoidal rule quadrature, and for a 
Chebyshev grid can be written as

where the label MS stands for momentum-shift formula.

Another prescription is given by DeWitt [19] which relates 
the phase shifts with the energy-levels shift produced in the sta-
tionary states of a system bound in a large spherical box, when 
a finite-range perturbation is introduced. This is formulated in 
the following way

where $\Delta E_n$ is the shift from the unperturbed to the perturbed 
energy levels and $\Delta E$ is the separation between levels in the 
unperturbed system. In terms of momentum-grid points the 
energy-shift (ES) formula reads

\[
\delta_n^{\text{ES}} = -\pi \frac{\sqrt{p_n^2 + m^2} - \sqrt{p_n^2 + m^2}}{p_n w_n}.
\]

Note that in the ultrarelativistic case, i.e. for very small 
masses Eqs. (57) and (56) are equivalent. This situation holds 
in the $\pi\pi$ scattering case at intermediate energies.

Based on DeWitt’s argument, we have generalized the for-

mula Eq. (56) to any momentum grid in the non-relativistic

\[ D_k = \begin{cases} \frac{w_k p_k^2}{4E_k} \frac{1}{E_{n-2E_k}} & \text{for } 1 \leq k \leq N \\ \frac{w_k}{4E_k} \frac{1}{E_{k-2E_k}} & \text{for } k = 0 \end{cases} \]  \tag{45}

\[
-\tan \delta^K_1(k_0) = \frac{\pi k_0}{8E_0} R_1(k_0, k_0, 2E_0). \tag{46}
\]

The question if we can check whether the calculated phase-
shift, or $\rho_{00} = R(k_0, k_0, 2E_0)$, at the observation point $k_0$ is 
isospectral or not, i.e. under the changes $\Delta V = i[\xi, H]$ on the 
grid requires to distinguish two relevant cases, depending on 
whether the observation point is included or not in the unitary 
transformation.

We sketch here a perturbative proof that isospectrality does 
not hold. In perturbation theory, and going to the barred basis 
we get to second order

\[
\bar{p}_{00} = \bar{V}_{00} + \sum_{k=1}^{N} D_k \bar{V}_{0k}^2 + D_0 \bar{V}_{00}^2 + O(V^3) \tag{47}
\]

so that because in any case $\Delta V_{00} = 0$ and

\[
\Delta V_{0k} = -\Delta V_{k0} = i \sum_{l=1}^{N} (\xi_{0l} \bar{H}_{lk} - \bar{H}_{0l} \xi_{lk}) + i (\xi_{0l} \bar{H}_{lk} - \bar{H}_{0l} \xi_{lk}) \tag{48}
\]

where $\bar{H}_{0l} = V_{0l}$ and $\bar{H}_{lk} = 2E_l \delta_{lk} + V_{lk}$ and we have

\[
\Delta \bar{p}_{00} = 2 \sum_{k=1}^{N} \frac{1}{2E_k - 2E_0} \bar{V}_{0k} \Delta V_{k0} + O(V^3) \tag{49}
\]

which is non-vanishing. Non-perturbatively we may take spe-
fic unitary transformations. While the observation points can 
be chosen arbitrarily, generally, we observe that close to the 
momentum grid points the phase-shifts are particularly unsta-
ble against unitary transformations either in the space $\mathcal{H}_N$ or 
$\mathcal{H}_{N+1}$. We have also analyzed the case of an unitary unipara-
metric family where infinitesimally $\Delta V = [H_0, V, H] \Delta s$ [40] 
using a grid of $N + 1$ observation points $k_n$ nested into the grid 
of $N$ momentum points $p_n$, i.e. $k_0 < k_1 < k_2 < k_3 \cdots < 
2N + 1$ dimensional space which leads to similar results.

where

H\Psi_n \equiv 2E_n \Psi_n + \sum_k w_k \frac{p_k^2}{4E_k} \Psi_k = \sqrt{s} \Psi_n, \tag{50}

\[ H \Psi_n \equiv 2E_n \Psi_n + \sum_k w_k \frac{p_k^2}{4E_k} \Psi_k = \sqrt{s} \Psi_n, \tag{50} \]

\[ H \Psi_n \equiv 2E_n \Psi_n + \sum_k w_k \frac{p_k^2}{4E_k} \Psi_k = \sqrt{s} \Psi_n, \tag{50} \]

4 The barred equations lead to identical eigenvalues.

5 We are assuming here that there are no bound states. For the bound state 
case, the formulas have to be modified in order to comply with Levinson’s 
theorem and in [28, 39].
with a small number of points. The generalization to any mo-
where \( \phi \) the interaction becomes milder when the interaction is coarse
grained. The most remarkable feature of these fits is the very long tail
of the interaction, particularly for the \( \pi\pi \)-wave, which reaches
the energy values the inversion method requires
\( N \) of grid points used in the calculation, namely,
\( N \) is the
momentum grid amounts to finding the variable that is distributed
equidistantly along the momentum grid.

Note that if we want the value of the phase-shift at \( N \) single
energy values the inversion method requires \( N \) matrix inver-
sions, whereas in the spectral shift methods the \( N \) phases are obtained at once in a single diagonalization.

V. NUMERICAL RESULTS

The purpose of this numerical analysis is to study the pre-
dictive power and the accuracy of the \( \phi \)-shift method in the
relativistic case of \( \pi\pi \) scattering, in a similar way as it was
done in the case of \( NN \)-scattering using a nonrelativistic toy model [30]. We will show here again that the \( \phi \)-shift method prescription is the one that best reproduces
the solution in the continuum. As we will see in our numerical
study, the method gives reliable predictions even for a grid
with a small number of points. The generalization to any momentum
grid amounts to finding the variable that is distributed
equidistantly along the momentum grid.

Form factors Eq. (58) are given in the Appendix A.

A. Separable models

For definiteness, we use the form of potentials determined
by the fit already carried out by H. Garcilazo and L. Mathe-
litsch [38] for the lowest partial waves using separable poten-
tials and upgrade the fitting parameters to the newest phases
reported by the most recent Madrid group 2011 analysis [41].
The most remarkable feature of these fits is the very long tail
of the interaction, particularly for the \( P \)-wave, which reaches
up to 10 GeV.

Long tails in momentum space indicate large strengths in
configuration space. In fact the effect has been observed in the
Marchenko approach to the inverse scattering problem [42].
The effect becomes milder when the interaction is coarse
gained.

The long-tails feature is not just an artifact of the fit, as for
instance the inverse scattering problem in coordinate space

\[ \delta_\phi = -\pi \frac{\Phi_n - \phi_n}{d \phi_n} = -\pi \Delta \phi_n, \]

where \( \phi_n = \frac{\pi}{2} (n - \frac{1}{2}) \), \( d \phi_n = \frac{\pi}{2} \), and the “distorted” angles \( \Phi_n \)
are calculated inverting Eqs. (22)-(25) replacing \( q_n \) by \( p_n \).

These three prescriptions, momentum-, energy- and \( \phi \)-shift, have been considered in the analysis of \( NN \)-scattering using a
nonrelativistic toy model [30]. We will show here again that the \( \phi \)-shift method prescription is the one that best reproduces
the solution in the continuum. As we will see in our numerical
study, the method gives reliable predictions even for a grid
with a small number of points. The generalization to any momentum
grid amounts to finding the variable that is distributed
equidistantly along the momentum grid.

Note that if we want the value of the phase-shift at \( N \) single
energy values the inversion method requires \( N \) matrix inver-
sions, whereas in the spectral shift methods the \( N \) phases are obtained at once in a single diagonalization.

\[ p \cot \delta_\phi (p) = -\frac{8 E_p}{\pi V_{\pi\pi}(p)} \left[ 1 - \int_0^\infty dq \frac{q^2}{4 E_q^2} \frac{V_{\pi\pi}(q,q)}{\sqrt{s} - 2 E_q} \right], \]
studied interval, while the other half are distributed along the long tail of the potential.

FIG. 2. (Color online) Phase shifts calculated using our \( \phi \)-shift prescription (blue dots) compared with the numerical fit (green, smooth line) and with the result obtained from the Lippmann-Schwinger equation (step-wise, orange line). Each column corresponds to the calculation made with a grid of \( N = 25, 50, \) and 100 points, respectively.

Both methods turn out to be very similar and accurate in the case of the \( Lf = S2, D0 \) and \( D2 \) waves. This is foreseeable, since while in the first two cases the phase shifts cover a wide range of values in a short energy interval, in the last three channels, the phase shifts remain rather small (\( \delta_{02}, \delta_{20} < \pm 30^\circ \) and \( \delta_{22} < 3^\circ \)) in the same energy range. Thus, perturbation
C. Comparison of the three different prescriptions

In this section we calculate phase shifts using the three different prescriptions presented in Section IV.

When using the $\phi$-shift, Eq. (57), or $E$-shift prescription, Eq. (56), we may represent the results as a function of the distorted momentum $P_n$, or as a function of the free momentum $p_n$. The phase shifts $\hat{\delta}(P_n)$ and $\hat{\delta}(p_n)$ will acquire the same values but will be horizontally displaced from each other by the momentum shift. This ambiguity does not arise in the $p$-shift case, since the phase shift is a function of the interacting momentum by construction.

Fig. 3 shows two lines for every $\pi\pi$-scattering channel. The upper row (in blue) shows the phase shifts calculated using the $\phi$-shift prescription, Eq. (57) while the lower row (in red) shows the phase shifts according to the energy-shift prescription, Eq. (56). The $p$-shift results are numerically almost identical in this case to the $E$-shift ones, and they are not depicted in an extra graphic. Phase shifts represented as a function of the transformed momentum $P_n$ are plotted using a darker line with round markers while phase shifts plotted as a function of the free momentum $p_n$ are given by a lighter line with square markers. All these lines are compared with the exact calculation represented by the green line without markers. In some cases, we have chosen a reduced interval, in such a way that the difference between lines is more visible.

We observe in Figure 3 that in all cases, the phase shifts represented as a function of the interacting momentum $P_n$ lie closer to the exact solution. This was already pointed out in the nonrelativistic case studied in [30]. Observing the first and third rows (blue) in Figure 3, we see that our $\phi$-shift results totally overlap the green line which is not even visible. The $E$-shift (as well as $p$-shift) prescription given in the second and forth rows (red) yields values that lie always below those provided by the momentum-shift one. In all cases, $\phi$- and $E$-shift, the phase shifts represented as a function of the free momentum $p_n$ (light line with square markers) appear displaced according to the momentum shift: to the right for attractive interactions, and to the left for repulsive ones. Indeed, the $P_n - p_n$ is negative for attractive interactions and positive for repulsive ones. Since the $p$-shift formula prescribes that the phase shift is a function of the interacting momentum, and the $E$-shift formula reproduces it in this case of very light masses, we assume that taking the interacting momentum as the independent variable is the most adequate option.

It was already explained in [30], that both the $E$- and $p$-shift prescriptions are actually an approximation of the $\phi$-shift formula. Indeed, the $E$-shift formula implies an equal-distance separation of energy levels, alike the $p$-shift formula implies an equal-distance separation in momentum space. The Gaussian separation of energy levels, alike the form of the phase shift, implies an equal-distance separation of momentum levels.

D. Heavy masses and non-equal masses

Figures 10-18 show the obtained results for $NN$-scattering, where the form factors for separable potentials are taken from [38] and are given in Appendix A. The phase shifts are plotted as a function of $T_{Lab}$.

The first row of each of these figures shows the $\phi$-shift result, compared with the LS results and with the exact solution for a grid of $N = 25$, 50, and 100 points, respectively. The second row shows the result obtained using the $\phi$-, $p$-, and $E$-shift, as labeled in the corner, for a momentum grid of $N = 50$ points. In this case, the proton mass is not negligible, and hence Eqs. (54) and (56) are no longer equivalent, and the numerical difference can be appreciated (see e.g. Figure 5). In analogy to what has been done in the $\pi\pi$ analysis, we use a darker like with round markers to represent the results when using the interacting momentum as the implicit independent variable, and a lighter line with square markers when we use the free momentum as the independent variable in $T_{Lab}$. We have selected in some cases an interval where the difference between lines is more visible.

In the studied interval, $0 \leq T_{Lab} \leq 300$, the phase shifts do not reach values higher than around 30 degrees, so that there are no abrupt changes in the curves and, as a consequence, the deviation from results obtained in one or other method is not significant.

Figures 10-18 show the phase shifts calculated for $\pi N$ scattering. Alike in the $NN$ case, Eqs. (54) and (56) are no equivalent due to the large mass of the proton involved. But one can hardly appreciate the difference from the numerical results due to the very small range of values that the phase shifts take in most of the channels, with the exception of the $P_{33}$ wave, which reaches from 0 to around 120 degrees.

VI. CONCLUSIONS

The analysis of hadronic interactions requires in many cases a numerical solution of the relativistic scattering problem, which from a quantum field theoretical point of view would be best formulated in terms of the 4D Bethe-Salpeter equation, but in practice one uses 3D reductions. This is most often done by placing the system in a finite momentum grid and proceeding to inverting the corresponding inhomogeneous scattering equation. In this paper we have analyzed the Kadyshevsky equation, which allows for a corresponding relativistic interpretation of the Schrödinger equation and is fully compatible with a field theoretical Hamiltonian formulation. As we have
We have generalized to the relativistic case a new prescription for calculating phase shifts. We have studied the predictive power of the momentum-shift and energy-shift prescriptions for calculating phase shifts. We have generalized to the relativistic case a new prescription based on an argument that holds for any momentum grid. The new prescription requires to find the variable that holds an equidistant space between points along the momentum grid. The chosen grid in this work is a Gauss–Chebyshev quadrature and the equal spacing occurs in the Chebyshev angle \( \phi = \frac{\pi}{2} (n - \frac{1}{2}) \). As it turns out, this prescription yields exceptionally good results, even in the case of a grid with a relatively small number of points.

Besides providing accurate isospectral phases even in rather coarse momentum grids, our \( \phi \)-shift formula is computationally cheaper than any conventional solution based on the matrix.

FIG. 3. (Color online) Phase shifts calculated using the \( \phi \)-shift, \( E \)-shift and \( p \)-shift methods for every channel in \( \pi\pi \)-scattering and compared with the exact solution (green, smooth line). The first and third lines (in blue) show the \( \phi \)-shift results and the second and forth lines (in red) show the \( E \)- or \( p \)-shift results, which are equal in this case due to the relativistic pion masses. In all cases the phase shifts are represented as a function of the distorted momentum (darker line with round markers), and as a function of the free momentum (lighter line with square markers). The calculation was made with a grid of \( N = 50 \) points.
We want to compute $N$ energy values of the phase-shift with a grid of $N$ points. We have a computational complexity of $N \times \mathcal{O}(N^2)$ because $N$-inversions are needed, whereas with the diagonalization method we have at once all phase-shifts with $\mathcal{O}(N^2)$ cost [23]. However, this happens at a price: while in our case the phases are computed at the interacting momenta, in the conventional solution the momenta are arbitrary.

All these findings are of special relevance for calculations that use a Hamiltonian framework. Indeed, many scattering studies are carried out within Lagrangian approaches, while the study of phase shifts in the context of a Hamiltonian formalism is rather sparse. It turns out, however, that the Hamiltonian formalism is very convenient or even necessary for certain purposes addressing renormalization issues [40].

The Kadyshevsky equation is very convenient in order to consider the three-body interaction problem. It is possible to couple the two-body interaction force into the three-body equation, in such a way that, for instance, a controlled knowledge of the $\pi\pi$-interaction, may lead to a precise description of $3\pi$.
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Appendix A: From factors. Model potentials

The form factors $g_{LL}$, with $L$ being the angular momentum and $I$ the isospin, in the case of $\pi\pi$ interaction are given by

$$g_{00}(p) = \frac{617.865 p^2}{(p^2 + 99.3951)^2} + \frac{423.64}{p^2 + 1034.75} . \quad (A1)$$
where all the potentials are attractive, i.e. the parameter $\eta = 1$ in Eq. (58), except the 02 and the 22 that are repulsive, i.e.

\[
g_{02}(p) = \frac{3.65 p^2}{(p^2 + 3.9601)^2} + \frac{175.7}{p^2 + 357.21},
\]

\[
g_{20}(p) = \frac{284.863 p^2}{(p^2 + 53.6235)^2},
\]

\[
g_{22}(p) = \frac{289.289 p^2}{(p^2 + 101.039)^2},
\]

For NN scattering we have for every $2s+1L_J$

\[
g_{11}(p) = p \left( \frac{132.237}{p^2 + 900.462} - \frac{5.11596}{p^2 + 21.9744} \right),
\]

\[
g_{02}(p) = \frac{3.65 p^2}{(p^2 + 3.9601)^2} + \frac{175.7}{p^2 + 357.21},
\]

\[
g_{20}(p) = \frac{284.863 p^2}{(p^2 + 53.6235)^2},
\]

\[
g_{22}(p) = \frac{289.289 p^2}{(p^2 + 101.039)^2},
\]

\[
g_{11}(p) = p \left( \frac{96.6852 p^2}{(p^2 + 8.72978)^3} + \frac{104.81}{(p^2 + 6.17934)^2} \right)
\]

\[
g_{11}(p) = p \left( \frac{139.976 p^2}{(p^2 + 4.3655)^3} + \frac{4.39386}{(p^2 + 0.877575)^2} \right)
\]

\[
g_{11}(p) = p \left( \frac{158.854 p^2}{(p^2 + 8.16363)^3} + \frac{15.1423}{(p^2 + 2.91507)^2} \right)
\]
\[ g_{1D_2}(p) = p^2 \left[ \frac{674.983}{(p^2 + 6.37134)^3} - \frac{179.268 p^2}{(p^2 + 2.74016)^4} \right] \]  
\[ g_{1D_2}(p) = p^2 \left[ \frac{513.691}{(p^2 + 4.44559)^3} - \frac{156.742 p^2}{(p^2 + 2.06874)^4} \right] \]  
\[ g_{3P_1}(p) = p^2 \left[ \frac{357.477}{(p^2 + 6.99909)^3} - \frac{111.479 p^2}{(p^2 + 4.26756)^4} \right] \]

and

\[ \eta_{1P_1} = \eta_{1P_1} = 1, \]
\[ \eta_{2P_2} = \eta_{1D_2} = \eta_{1D_2} = \eta_{1D_3} = -1. \]

Finally, the form factors for \( \pi N \) scattering are, for every \( L_{2S1/2} \) channel

\[ g_{S_1}(p) = \frac{14.6454}{p^2 + 12.2543}, \quad (A14) \]
\[ g_{S_3}(p) = \frac{95.4252}{p^2 + 30.9159} - \frac{3.13741}{p^2 + 1.83667}, \quad (A15) \]
\[ g_{P_3}(p) = p \left( \frac{36.8052}{p^2 + 102.726} + \frac{0.0867424}{p^2 + 0.226963} \right), \quad (A16) \]
\[ g_{P_3}(p) = p \left( \frac{10.4023}{p^2 + 15.7088} + \frac{2.31101}{p^2 + 31.1786} \right), \quad (A17) \]
\[ g_{P_3}(p) = \frac{13.079 p}{p^2 + 12.222}, \quad (A18) \]
\[ g_{D_{13}}(p) = \frac{364.057p^2}{(p^2 + 49.925)^2}, \]  \quad (A19)  
\[ g_{D_{15}}(p) = \frac{10.8919p^2}{(p^2 + 6.79962)^2}, \]  \quad (A20)  
\[ g_{D_{33}}(p) = \frac{2.18078p^2}{(p^2 + 3.20603)^2}, \]  \quad (A21)

\[ g_{D_{55}}(p) = \frac{7.52545p^2}{(p^2 + 5.20257)^2}, \]  \quad (A22)

In all cases the parameters have units of fm$^{-1}$ or fm$^{-2}$ as corresponds in such a way that the form factors are dimensionless.

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FIG. 15. The same as in Figure 4 but for $\pi N$ scattering in the $D_{13}$ channel.

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FIG. 16. The same as in Figure 11 but for $\pi N$ scattering in the $D_{15}$ channel.

FIG. 17. The same as in Figure 11 but for $\pi N$ scattering in the $D_{33}$ channel.

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