The scattering matrix from bound state solutions

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Abstract. Two integral relations, that have been recently derived from the Kohn variational principle (KVP), are used to describe scattering states. In usual applications the variational scattering wave function requires the explicit form of its asymptotic behavior. This is not the case when the integral relations are applied since, due to their short range nature, the only condition is that the scattering wave function \( \Psi \) be the solution of \((H-E)\Psi=0\) in the internal region. In order to show the applicability of the method, two examples are analyzed as the computation of phase-shifts from bound state type wave functions in the \( A=2 \) using a model potential. As a last example we discuss the use of the integral relations in the \( A=3 \) system using a realistic nucleon-nucleon potential.

1. Introduction
Much of the information of the nucleon-nucleon \((NN)\) interaction is obtained from the study of \( p-p \) and \( n-p \) scattering. Specific interaction models reproduce the available \( NN \) data with a \( \chi^2 \) per datum close to one. The application of these models to study the nuclear dynamics in systems with \( A > 2 \) is limited from our capability of solving the corresponding Schrödinger equation. For example, the fact that the spectrum of each hydrogen and helium isotope has only one bound state in the mass region \( A = 2 - 4 \) and the \( A = 5 \) nucleus does not exist, limits the applicability of bound state methods in the study of these nuclei to a few states. In Ref. [1] a detailed study of the three-nucleon bound states has been done, whereas a similar analysis in the case of \(^4\)He can be found in Refs. [2, 3]. In recent years much of the study in the three-nucleon system has been done in the three-nucleon continuum (see Refs. [4, 5] and references therein). Results in the four-body system have been obtained so far in the energy region below the breakup in three particles [6, 7].

Well established methods to treat both, bound and scattering states, are the solution of the Faddeev equations \((A=3)\) or Faddeev-Yakubovsky equations \((A=4)\) in configuration or momentum space and the Hyperspherical Harmonic (HH) expansion in conjunction with the Kohn variational principle (KVP). These methods have proven to be of great accuracy. They have been tested through different benchmarks [8, 9]. On the other hand, many other methods are presently used to describe bound states: for example the Green Function Montecarlo (GFMC) and No Core Shell Model (NCSM) methods have been used in nuclei up to \( A = 10 \) and \( A = 12 \) respectively [10, 11]. Attempts to use these methods in the description of scattering states recently appeared [12, 13].

The possibility of employing bound state techniques to describe scattering states has always attracted particular attention [14]. Also recently continuum-discretized states obtained from
the stochastic variational method have been used to study $\alpha + n$ scattering [15]. In those two approaches the tangent of the phase-shift results a quotient of two numbers. In the former the numerator and denominator are obtained from two integral relations after projecting the Schrödinger equation, whereas in the latter the numerator results from an integral relation derived by means of the Green’s function formalism and the denominator from the normalization of the continuum-discretized state.

Recently two integral relations have been derived from the KVP [16]. It has been shown that starting from the KVP, the tangent of the phase-shift can be expressed in a form of a quotient where both, the numerator and the denominator, are given as two integral relations. This is similar to what was proposed in Ref. [14], however the variational character of the quotient and its strict relation with the KVP were not recognized. In fact, it is this characteristic that makes possible many different and interesting applications of the integral relations. Accordingly, in the present study we would like to discuss some specific examples. We will show that the integral relations can be used to compute phase-shifts from bound-state-like functions. We start our analysis from the simplest case, the $A = 2$ system, using a model potential. Then, using a semirealistic interaction, $n - d$ as well as $p - d$ scattering are considered. This is of particular interest since $p - d$ scattering has been a subject of intense investigations. A second application of the integral relations regards the possibility of determining $p - d$ phase-shifts from a calculation in which the Coulomb potential has been screened. Finally, as a third application, we will discuss the use of the integral relations in which more than one channel is open. All these examples serve to demonstrate the general validity of the KVP formulated in terms of integral relations. Due to their short-range nature, they are determined by the wave function in the interaction region and not from its explicit asymptotic behavior. This means that each wave function $\Psi$ verifying $(H - E)\Psi = 0$ in the interaction region can be used to determine the corresponding scattering amplitude even if its asymptotic behavior is not the physical one.

2. Integral relations from the Kohn variational principle

Following Ref. [16] we give a brief derivation of the integral relations. Let us first consider a two-body system interacting through a short-range potential $V(r)$ at the center of mass energy $E$ in a relative angular momentum state $l = 0$. The solution of the Schrödinger equation in configuration space ($m$ is twice the reduced mass),

$$(H - E)\Psi(r) = (-\frac{\hbar^2}{m}\nabla^2 + V - E)\Psi(r) = 0 ,$$

can be obtained after specifying the corresponding boundary conditions. For $E > 0$, with $k^2 = E/((\hbar^2/m)$ and assuming a short-range potential $V$, $\Psi(r) = \phi(r)/\sqrt{4\pi}$ and

$$\phi(r \to \infty) \longrightarrow \sqrt{k} \left[ A \frac{\sin(kr)}{kr} + B \frac{\cos(kr)}{kr} \right] .$$

from which one gets $\Psi \to AF + BG$, where

$$F = \sqrt{\frac{k \sin(kr)}{4\pi kr}} \quad \text{and} \quad G = \sqrt{\frac{k \cos(kr)}{4\pi kr}} .$$

Using the normalization condition

$$\frac{m}{\hbar^2} \left[ < F|H - E|G > - < G|H - E|F > \right] = 1 .$$
and assuming that $\Psi$ is an exact solution of Eq.(1), the wave function verifies the following integral relations:

$$-rac{m}{\hbar^2} < \Psi | H - E | \tilde{G} > = B,$$
$$\frac{m}{\hbar^2} < \Psi | H - E | \tilde{G} > = A,$$
$$\tan \delta = \frac{B}{A}.$$  \hspace{1cm} (5)

In the above expressions we have introduced the regularized function $\tilde{G} = f_{reg}G$ with the property $|\tilde{G}(r = 0)| < \infty$ and $\tilde{G} = G$ outside the interaction region. A possible choice is

$$\tilde{G} = \sqrt{k^4 \pi \cos(kr) k^2 r (1 - e^{-\gamma r})},$$  \hspace{1cm} (6)

with $\gamma$ being a non linear parameter which will be discussed below. Values verifying $\gamma > 1/r_0$, with $r_0$ the range of the potential, could be appropriate.

In practical cases the solution of the Schrödinger equation is obtained numerically. Then, $\tan \delta$ is extracted from $\phi(r)$ analyzing its behavior outside the range of the potential. The equivalence between the extracted value and that one obtained from the integral relations defines the accuracy of the numerical computation. A relative difference of the order of $10^{-7}$ of the two values is usually achieved using standard numerical techniques to solve the differential equation and to compute the two one-dimensional integrals. To be noticed the short range character of the integral relations. This means that the phase-shift is determined by the internal structure of the wave function.

In the following we demonstrate that the relation $\tan \delta = B/A$, which is an exact relation when the exact wave function $\Psi$ is used in Eq (5), can be considered accurate up to second order when a trial wave function is used, as it has a strict connection with the Kohn variational principle. The connection of the integral relations with the KVP is straightforward. Defining a trial wave function $\Psi_t$ as

$$\Psi_t = \Psi_c + AF + B \tilde{G} ,$$  \hspace{1cm} (7)

with $\Psi_c \to 0$ as $r \to \infty$, the condition $\Psi_t \to AF + B G$ as $r \to \infty$ is fulfilled. The KVP states that the second order estimate for $\tan \delta$ is

$$[\tan \delta]^{2nd} = \tan \delta - \frac{m}{\hbar^2} < \frac{1}{A} \Psi_t | H - E | \frac{1}{A} \Psi_t > .$$  \hspace{1cm} (8)

The above functional is stationary with respect to variations on $\Psi_c$ and $\tan \delta$. As shown in Ref. [16] it can be given as

$$B^{2nd} = -\frac{m}{\hbar^2} < \Psi_t | H - E | F > ,$$
$$A = \frac{m}{\hbar^2} < \Psi_t | H - E | \tilde{G} > ,$$
$$[\tan \delta]^{2nd} = B^{2nd} / A .$$  \hspace{1cm} (9)

These equations extend the validity of the integral relations, given in Eq.(5) for the exact wave functions, to trial wave functions. Moreover these relations are valid for generic values of the number of particles. In the case in which more than one channel is open the coefficients $A$ and $B$ of the above equations correspond to matrices

$$B^{2nd}_{ij} = -\frac{m}{\hbar^2} < \Psi_t | H - E | F_j > ,$$
$$A_{ij} = \frac{m}{\hbar^2} < \Psi_t | H - E | \tilde{G}_j > ,$$
$$R^{2nd} = A^{-1} B^{2nd} .$$  \hspace{1cm} (10)
with $R^2_{\text{2nd}}$ the second order estimate of the scattering matrix whose eigenvalues are the phase shifts and the indeces $(i, j)$ indicate the different asymptotic configurations accessible at the specific energy under consideration.

To be noticed that $F, \tilde{G}$ are solutions of the Schrödinger equation in the asymptotic region, therefore $(H - E)F \to 0$ and $(H - E)\tilde{G} \to 0$ as the distance between the particles increases. As a consequence the decomposition of $\Psi_t$ in the three terms of Eq. (7) can be considered formal since, due to the short-range character of the relation integrals, it is sufficient for the trial wave function to be a solution of $(H - E)\Psi_t = 0$ in the interaction region, without an explicit indication of its asymptotic behavior. This fact, together with the variational character of the relations allows for a number of applications to be discussed in the next section.

3. Application of the integral relations

We first discuss an application of the integral relations of Eq. (9) to a two-body system. To make contact with the results given in Refs. [16, 17], we use a central, $s$-wave gaussian potential

$$V(r) = -V_0 \exp \left(-r^2/r_0^2\right) ,$$

with $V_0 = -51.5$ MeV, $r_0 = 1.6$ fm and $\hbar^2/m = 41.4696$ MeV fm$^2$. This potential has a shallow $L = 0$ bound state with energy $E_{2B} = -0.397743$ MeV.

We introduce the orthogonal basis

$$\phi_m = L_m^{(2)}(z) \exp \left(-z/2\right) ,$$

with $L_m$ a (normalized) Laguerre polynomial and $z = \beta r$, where $\beta$ is a nonlinear parameter, to expand the wave function of the system

$$\Psi_0 = \sum_{m=0}^{M-1} a^0_m \phi_m .$$

We solve the eigenvalue problem of $H$ for different dimensions $M$ of the basis. The variational principle states that

$$E_0 = \langle \Psi_0 | H | \Psi_0 \rangle \geq E_{2B} ,$$

with the equality valid when $M \to \infty$. The nonlinear parameter $\beta$ can be fixed to improve the convergence properties of the basis. In fact, for each value of $M$ there is a value of $\beta$ that minimizes the energy. Increasing $M$, the minimum of the energy becomes less and less dependent on $\beta$ resulting in a plateau. Increasing further the dimension of the basis, the extension of the plateau increases as well, without any appreciable improvement in the eigenvalue, indicating that the convergence has been reached to a certain accuracy. At each step $\Psi_0$ represents a first order estimate of the exact bound state wave function. Since, in our example, the system has only one bound state, with appropriate values of $M$ and $\beta$, the diagonalization of $H$ results in one negative eigenvalue $E_0$ and $M - 1$ positive eigenvalues $E_j$ ($j = 1, \ldots, M - 1$). The corresponding wave functions

$$\Psi_j = \sum_{m=0}^{M-1} a^j_m \phi_m \quad j = 1, \ldots, M - 1 ,$$

are approximate solutions of $(H - E_j)\Psi_j = 0$ in the interaction region. As $r \to \infty$ they go to zero exponentially and therefore they do not represent physical scattering states. The eigenvectors can be used to compute the integral relations of Eq. (9) and to calculate the second order estimate of the phase-shifts $\delta_j$ at the specific energies $E_j$. This analysis is shown in table 1 in which the non linear parameter $\beta$ of the Laguerre basis has been chosen to be 1.2 fm$^{-1}$. In
the first row of the table the ground state energy is given for different values of the number $M$ of Laguerre polynomials. The stability of $E_0$ at the level of $1$ keV is achieved already with $M = 20$. For a given value of $M$, $E_j$, with $j = 1, 2, 3$, are the first three positive eigenvalues. The eigenvectors corresponding to positive energies approximate the scattering states at these specific energies. Since the lowest scattering state appears at zero energy, none of the positive eigenvalues can reach this value for any finite values of $M$. We observe that the eigenvalues diminish as $M$ increases. Defining $k_j^2 = \frac{\bar{m}}{\hbar^2} E_j$, the second order estimate for the phase shift at each energy and at each value of $M$ is obtained as

\[
-\frac{m}{\hbar^2} < \Psi_j | H - E | F_j > = B_j \quad \text{with} \quad F_j = \sqrt{\frac{k_j \sin(k_j r)}{4\pi k_j r}}
\]

\[
\frac{m}{\hbar^2} < \Psi_j | H - E | \tilde{G}_j > = A_j \quad \text{with} \quad \tilde{G}_j = f_{reg} \sqrt{\frac{k_j \cos(k_j r)}{4\pi k_j r}}
\]

\[
|\tan \delta_j|^{2nd} = \frac{B_j}{A_j}.
\]

On the other hand, as we are considering the $A = 2$ system, at each specific energy value $E_j$ the phase shift $\tan \delta_j$ can be obtained by solving the Schrödinger equation numerically. The two values, $|\tan \delta_j|^{2nd}$ and $\tan \delta_j$, are given in the table 1 at the corresponding energies as a function of $M$. We observe that, as $M$ increases, the relative difference between the variational estimate and the exact value reduces, for example at $M = 40$ it is about $10^{-6}$. In fact, as $M$ increases, each eigenvector gives a better representation of the exact wave function in the internal region and the second order estimates, $|\tan \delta_j|^{2nd}$ approach the exact result.

| Table 1. | The two-nucleon bound state $E_0$ and the first three positive eigenvalues $E_j$ ($j = 1, 3$), as a function of the number of Laguerre polynomials $M$. The second order estimates, $|\tan \delta_j|^{2nd}$, obtained applying the integral relations are given in each case and compared to the exact results, $\tan \delta_j$. |
|----------|-----------------|-----------------|-----------------|-----------------|
| $E_0$    | $-0.395079$     | $-0.397740$     | $-0.397743$     | $-0.397743$     |
| $E_1$    | $0.536349$      | $0.116356$      | $0.048091$      | $0.026008$      |
| $|\tan \delta_1|^{2nd}$ | $-1.507280$ | $-0.622242$ | $-0.392005$ | $-0.286479$ |
| $\tan \delta_1$ | $-1.522377$ | $-0.621938$ | $-0.392021$ | $-0.286480$ |
| $E_2$    | $1.984580$      | $0.449655$      | $0.190019$      | $0.103503$      |
| $|\tan \delta_2|^{2nd}$ | $-5.919685$ | $-1.353736$ | $-0.812313$ | $-0.584389$ |
| $\tan \delta_2$ | $-5.703495$ | $-1.354691$ | $-0.812270$ | $-0.584388$ |
| $E_3$    | $4.512635$      | $0.994433$      | $0.423117$      | $0.231645$      |
| $|\tan \delta_3|^{2nd}$ | $13.998124$ | $-2.451174$ | $-1.302799$ | $-0.908128$ |
| $\tan \delta_3$ | $12.684474$ | $-2.448343$ | $-1.302887$ | $-0.908131$ |

In the following application the study of the integral relations is extended to describe a $2 + 1$ collision in the three-body system, below the breakup threshold into three particles. Following Refs. [18, 19, 20, 21] a general three-nucleon bound state can be expand in terms of the hyperspherical harmonic basis as

\[
\Psi_n = \sum_{\alpha, K, m} A^n_{\alpha, K, m} |\alpha, K, m >,
\]
where the index $n$ indicates the level of the state with energy $E_n$ and $|\alpha, K, m>$ is a totally antisymmetric element of the expansion basis for the $A = 3$ system. The linear coefficients $A_{\alpha, K, m}$ of the wave function and the energy of the state are obtained by solving the following generalized eigenvalue problem

$$\sum_{\alpha', K', m'} A_{\alpha', K', m'}^n < \alpha, K, m | H - E_n | \alpha', K', m' > = 0 .$$  \hspace{1cm} (18)

Considering a realistic nucleon-nucleon interaction as the AV14 potential and focussing in the $J^\pi = 1/2^+$ state, the lowest solution of the eigenvalue problem ($n = 0$) is the triton bound state. A certain number of negative eigenvalues verifying $E_n > E_d$ (with $E_d$ the deuteron energy) also appear. Defining the positive energy $E$ in the continuum spectrum corresponding to the two possible couplings of the total spin $J$, $E$ though asymptotically they go to zero. The lowest eigenvalue $E_0$ of the wave function and the energy of the state are obtained by solving the following integral relations of Eq.(9) depend on the internal part of the wave function and therefore integral relations of Eq.(9) depend on the internal part of the wave function and therefore

$$E_n = \frac{1}{2} \sum_{i,j} \sum_{\alpha, K} \sum_{L, S, J} | H_n | \Omega^0_{ij} >,$$

$$R = A^{-1} [B],$$  \hspace{1cm} (19)

where $i, j$ indicate either the two solutions, $\Psi^1$ and $\Psi^2$, and the two possible values of the set of quantum numbers ($L, S, J$) in $J = 1/2^\pm$. The regular and irregular asymptotic functions $\Omega^0_{ij}$ and $\Omega^1_{ij}$ are defined as

$$\Omega_{L,S,J}(x_i, y_i) = \sum_{l=0,2} w_{l}(x_i) R_{L}^1(y_i) \left\{ \left[ Y_{l}(\vec{x}_i) s_{\alpha}^{jk} \right]_{1}^1 \left[ Y_{L}(\vec{y}_i) \right]_{1}^1 \right\}_{J,J_z} [n^{\alpha}_{\lambda}]^{TT_2},$$  \hspace{1cm} (20)

where $w_{l}(x_i)$ is the $l = 0, 2$ deuteron wave function, $s_{\alpha}^{jk} = 1, t_{\alpha}^{jk} = 0$, and $L$ is the relative angular momentum of the deuteron and the incident nucleon. The superscript $\lambda$ indicates the regular ($\lambda = 0$) or the irregular ($\lambda = 1$) solution of the Schrödinger equation in the asymptotic region. It should be noticed that the irregular solution has been opportunely regularized at the origin

$$R_{L}^1(y) = (1 - e^{-\gamma r_{Nd}})^{L+1} G_{L}(y),$$  \hspace{1cm} (21)

where $r_{Nd} = (\sqrt{3}/2) y$ is the nucleon-deuteron separation and the parameter $\gamma$ is fixed requiring that $R_{L}^1(y) \equiv G_{L}(y)$ asymptotically.

Results of phase-shifts and mixing parameters for the $n - d$ system, calculated using the AV14 $NN$ potential, are presented for the $J^\pi = 1/2^+$ state in figure 1 at the three selected energies $E_{lab} = 1, 2, 3$ MeV. The stability of the results with $\gamma$, the regularization parameter
introduced in Eq.(21), is chosen as a convergence criterion. This criterion has been discussed in Refs. [16, 22] and essentially it establishes the quality of $\Psi_i^n$ as solution of $(H - E_n)\Psi_i^n = 0$. In fact, if $\Psi_i^n$ is a good solution, the integrals of Eq.(19) are largely independent of $\gamma$. The results are compared to the benchmark of Ref. [8] given in the figures as a red line. The results of the application of Eq.(19) are shown as filled circles corresponding to values of $\gamma$ varying from $0.25 \text{ fm}^{-1}$ to $1.25 \text{ fm}^{-1}$. We can observe a good stability on this interval and, furthermore, the results are in very good agreement with those of Ref [8].

Figure 1. (Color online) The $n-d J^\pi = 1/2^+$ phase-shifts and mixing parameters as a function of the regularization parameter $\gamma$ at the three indicated energies. The red line corresponds to the results of Ref. [8].

4. Conclusions
In this work the elastic scattering matrix has been determined using bound-state-like wave functions. To this end two integral relations derived from the KVP have been used. Initially, these integral relations were derived in Ref. [16] in order to extract phase shifts from the solutions calculated using the hyperspherical adiabatic expansion in the three-nucleon system. Here applications to elastic scattering of a nucleon on a deuteron ($A = 3$) below the breakup threshold, using realistic nucleon-nucleon potentials has been discussed. In particular two
solutions at the same energy have to be determined corresponding to the different possible asymptotic configurations of the system. The obtained results are in close agreement with those presented in the \( A = 3 \) benchmark of Ref. [8]. A more detailed analysis of the use of the integral relations in the \( A = 3, 4 \) systems is in progress [23].

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