

Continuum discretization using orthogonal polynomials

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A method for discretizing the continuum by using a transformed harmonic oscillator basis has recently been presented [Phys. Rev. A **63**, 052111 (2001)]. In the present paper, we propose a generalization of that formalism which does not rely on the harmonic oscillator for the inclusion of the continuum in the study of weakly bound systems. In particular, we construct wave functions that represent the continuum by making use of families of orthogonal polynomials whose weight function is the square of the ground state wave function, expressed in terms of a suitably scaled variable. As an illustration, the formalism is applied to one-dimensional Morse, Pöschl-Teller, and square well potentials. We show how the method can deal with potentials having several bound states, and for the square well case we present a comparison of the discretized and exact continuum wave functions.

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I. INTRODUCTION

For any realistic composite quantum-mechanical system (atoms, molecules, nuclei, etc.) the treatment of the continuous part of the spectrum is a difficult task. This is especially so in the case of weakly bound systems, when both bound and unbound states have to be treated on equal footing. The continuum wave functions depend on a continuously varying parameter (the energy or the wave number) and are not normalizable, which makes them awkward for actual applications. Nevertheless, in some cases the exact non-normalizable continuum wave functions can be explicitly used in the calculation. This is the case for the evaluation of excitation functions for an operator that connects a bound state with the continuum states of a system. In this situation, the bound character of the state allows for an explicit evaluation of the matrix elements. This is also the case in reaction calculations in a distorted-wave Born approximation approach. The transition amplitudes can be calculated from the matrix element of the relevant interaction between the initial bound state and the final unbound state.

However, in general, the explicit inclusion of the continuum states in structure or reaction calculations requires a discretization of the continuum. Thus, the continuum is substituted by a discrete set of normalizable states which becomes a complete set as the number of states considered tends to infinity. It is expected that a finite number of these discrete states will appropriately model the effect of the true continuum. This can be checked by investigating the convergence of the calculation as the number of discrete states included in the basis is increased.

Different methods are used to generate a discrete basis for the continuum. One of them is to use the *R*-matrix formalism [1]. This is a successful procedure but for realistic systems is computationally very demanding. Another possibility for discretizing the continuum is the use of a Sturmian basis. Given a potential, it is composed of the bound eigenstates obtained by rescaling the interaction under the constraint that they have the same binding energy as the original bound state

[2–4]. This basis is complete within the range of the potential. The convergence of this basis is good for short range operators, with a similar range as the binding potential, which couple the ground state to states with relatively high excitation energy. However, the Sturmian basis is not adequate for describing the low energy part of the continuum, which can be very important for weakly bound systems.

An analytical basis, such as the harmonic oscillator (HO) basis, can be used to describe both the bound and continuum states of the system. However, in order to describe accurately the ground state of a weakly bound system, many HO wave functions are required. This is due to the fact that the tail of the bound wave function is an exponential, while the tails of the HO wave functions have Gaussian behavior. An alternative is to use the transformed harmonic oscillator (THO) method [5], which is based on a general local scale transformation (LST) to the harmonic oscillator functions [6–10]. The transformed harmonic oscillator basis retains the simplicity of the harmonic oscillator expansion and includes the correct asymptotic behavior for the ground state. We have applied the THO method to describe bound and continuum states of weakly bound systems [5].

In this work, we introduce the orthogonal polynomial (OP) method, which is a generalization of the THO method. In the same spirit as in Ref. [5], a discrete basis is introduced to take into account the continuum; however, this basis is not necessarily related to transformed harmonic oscillator wave functions. Moreover, we show that the OP method can be applied with an arbitrary choice of the local scale transformation.

In our previous paper we considered potentials with just one bound state. Here we show how the method can be successfully applied to the multibound case. We show that the bound states are accurately described as we enlarge the dimension of the basis. In addition, we compare the discrete states that describe the continuum in the OP bases with the actual continuum states.

The paper is structured as follows. In Sec. II, the general orthogonal polynomial method is presented. In Sec. III, par-

ticular cases of the OP method are described, including the THO method. In Sec. IV the application of the formalism presented in the preceding sections is worked out for several one-dimensional (1D) potentials. Section V is devoted to a comparison of the wave functions representing the continuum obtained with this formalism with the actual continuum wave functions. Finally, in Sec. VI the outlook and conclusions of this work are presented.

II. THE GENERAL ORTHOGONAL POLYNOMIAL METHOD FOR ONE-DIMENSIONAL PROBLEMS

We consider a one-dimensional Hamiltonian that in appropriate units can be written as

$$h = -\frac{1}{2} \frac{d^2}{dx^2} + v(x), \quad (1)$$

h , x , and $v(x)$ here are dimensionless quantities, $x = \alpha r$, where r is the physical coordinate, and $h = H\mu/\hbar^2\alpha^2$, where H is the Hamiltonian.

The starting point of the proposed approach is to assume that the ground state wave function $\varphi_0(x)$ is known, either analytically or numerically,

$$h\varphi_0(x) = e_0\varphi_0(x). \quad (2)$$

Then a weight function $\omega(s)$ is defined as

$$\omega(s) = \frac{dx}{ds} |\varphi_0(x)|^2, \quad (3)$$

where $s(x)$ is an arbitrary function that has to be continuous, single valued, and monotonically increasing or decreasing, taking values in an interval $[a, b]$. Having defined the interval and the weight function, one can construct a family of orthogonal polynomials $\{P_n(s); n=0, 1, 2, \dots\}$ that satisfy

$$\int_a^b ds \omega(s) P_n(s) P_m(s) = \frac{1}{\mathcal{N}_n \mathcal{N}_m} \delta_{n,m}. \quad (4)$$

From these polynomials and the ground state wave function, it is straightforward to construct a set of orthonormal wave functions

$$\phi_m(x) = \langle x | \text{OP}, m \rangle = \mathcal{N}_m \varphi_0(x) P_m(s(x)) \quad (5)$$

that satisfy

$$\int_{-\infty}^{+\infty} dx \phi_m(x) \phi_n(x) = \delta_{n,m}. \quad (6)$$

The functions $\phi_n(x)$, excepting $\phi_0(x)$ which is actually the ground state wave function, are not eigenfunctions of the Hamiltonian, but constitute a basis in which the Hamiltonian can be diagonalized. This basis, which has infinite elements, can be truncated to a few states, provided that the appropriateness of the truncation is checked. In the particular case of weakly bound systems the Hamiltonian has few bound states and a continuum of unbound non-normalizable states. This

procedure allows for a convenient description of both bound and continuum states by means of a finite number of normalizable states.

In previous work [5,11,12] the weight function $\omega(x)$ was chosen in such a way that the local scale transformation $s(x)$ mapped the ground state wave function $\varphi_0(x)$ into the harmonic oscillator ground state wave function $\phi_0^{HO}(s)$. In this case, the polynomials $P_n(x)$ were related to the Hermite polynomials. The proposed method for continuum discretization, called the transformed harmonic oscillator, seemed to be necessarily linked to the harmonic oscillator. One of the purposes of this paper is to point out that the proposed method is not necessarily associated with the harmonic oscillator, although the THO method can be a good option. Different scale transformations $s(x)$ provide different discrete bases to diagonalize the Hamiltonian. The optimal selection for $s(x)$ depends on the particular observable that should be more accurately described.

Once the scale transformation $s(x)$ is chosen, the discrete basis $\phi_n = |\text{OP}; n\rangle$ can be generated and we can evaluate the matrix elements of the Hamiltonian h in this basis:

$$\langle \text{OP}, n | (h - e_0) | \text{OP}, m \rangle = \int dx \phi_n(x) (h - e_0) \phi_m(x). \quad (7)$$

We can take into account Eq. (5) and that $(h - e_0)\phi_0(x) = 0$ to write

$$\begin{aligned} \langle \text{OP}, n | (h - e_0) | \text{OP}, m \rangle &= \frac{\mathcal{N}_n \mathcal{N}_m}{2} \int dx \varphi_0(x) [P_n(s(x)), \\ &[(h - e_0), P_m(s(x))]] \varphi_0(x). \end{aligned} \quad (8)$$

The double commutator is independent of the potential and gives

$$[P_n(s(x)), [(h - e_0), P_m(s(x))]] = \frac{dP_n(s(x))}{dx} \frac{dP_m(s(x))}{dx}. \quad (9)$$

Taking this into account one gets

$$\begin{aligned} \langle \text{OP}, n | (h - e_0) | \text{OP}, m \rangle &= \frac{\mathcal{N}_n \mathcal{N}_m}{2} \int dx |\varphi_0(x)|^2 \frac{dP_n(s(x))}{dx} \frac{dP_m(s(x))}{dx}, \end{aligned} \quad (10)$$

which can be written in terms of the variable s :

$$\begin{aligned} \langle \text{OP}, n | (h - e_0) | \text{OP}, m \rangle &= \frac{\mathcal{N}_n \mathcal{N}_m}{2} \int ds \left(\frac{ds}{dx} \right)^2 \omega(s) \frac{dP_n(s)}{ds} \frac{dP_m(s)}{ds}. \end{aligned} \quad (11)$$

Once the LST $s(x)$ is selected, this expression can be easily evaluated using Gaussian quadratures. Note that the only information required is the derivative of the function $s(x)$, evaluated at the points x_n that define the quadrature.

The matrix elements with $n=0$ or $m=0$ vanish. This is due to the fact that the state of $n=0$ is an eigenstate of the Hamiltonian. Let us consider that we diagonalize the Hamil-

tonian in an N -dimensional basis of OP states, from $i=0$ to $i=N-1$. The eigenstates of the Hamiltonian, in this restricted basis, are given by

$$|N,0\rangle = |\text{OP},0\rangle, \quad (12)$$

$$|N,i\rangle = \sum_{j=1}^{N-1} |\text{OP},j\rangle \langle \text{OP},j|N,i\rangle, \quad (13)$$

where the states $|N,i\rangle$ ($i=1, \dots, N-1$) represent states different from the ground state in the truncated N -dimensional OP basis. They can be expressed in the x representation as

$$\langle x|N,i\rangle = \psi_i^N(x) = N_i P_i^{N-1}(s(x)) \phi_0(x), \quad (14)$$

where $P_i^{N-1}(s)$ is a polynomial given by

$$P_i^{N-1}(s) = \sum_{j=1}^{N-1} \mathcal{N}_j P_j(s) \langle \text{OP},j|N,i\rangle. \quad (15)$$

The diagonalization of the Hamiltonian in the OP basis, Eq. (11), provides the eigenvalues and eigenfunctions, Eqs. (14),(15). With them we can proceed to evaluate the matrix elements of any arbitrary local operator $O(x)$ that connects bound with unbound states. In this paper, we concentrate on the following observables: (a) total strength: $S(O;N) = \sum_i |\langle N,i|O|N,0\rangle|^2$; (b) energy weighted sum rule: $E_W(O;N) = \sum_i (e_i^N - e_0) |\langle N,i|O|N,0\rangle|^2$; and, (c) polarizability: $P(O;N) = \sum_{i \neq 0} (e_i^N - e_0)^{-1} |\langle N,i|O|N,0\rangle|^2$.

For all of them the exact result, including the complete set of bound and continuum states, can be calculated. Thus, we can compare the convergence of the OP results as the dimension of the basis is increased.

In the following sections we consider as an example different local scale transformations for multibound one-dimensional potentials: the Morse, Pöschl-Teller, and semi-infinite square well potentials. We examine in all cases the convergence of the bound states and global observables as the number of OP states included in the calculation is increased. With regard to the form of the operators $O(x)$, we consider two different cases as in the previous paper. First, we take $O(x)=x$ as an example of a long range operator, suited to describe the effects of external fields, such as the Coulomb field. Note that for an ideal polar diatomic molecule composed of two ions of definite charge, x is proportional to the electric dipole operator. In the second place, we consider a short range operator $O(x)=v(x)$, which could describe possible effects of internal correlations with a range similar to the potential.

In addition, in the case of the semi-infinite square well, we will show a comparison of the wave functions that represent the continuum provided by this method with the actual continuum wave functions.

III. SPECIAL CASES OF THE ORTHOGONAL POLYNOMIAL METHOD

In this section we work out different selections for the local scale transformation $s(x)$ that will be applied to various

potentials in the next section. These will be special cases of the general OP method.

A. Transformed harmonic oscillator method

In this case, the local scale transformation is selected so that it transforms the ground state wave function of interest into the ground state wave function of a harmonic oscillator,

$$\int_{-\infty}^x |\varphi_0(x')|^2 dx' = \int_{-\infty}^s |\phi_0^{HO}(s')|^2 ds' = \frac{1 + \text{erf}(s)}{2}. \quad (16)$$

Direct integration of Eq. (16) provides the function $s(x)$. Once the $s(x)$ function is computed, Eqs. (3)–(5) define the THO basis. In this case the relevant polynomials are Hermite,

$$\phi_n^{THO}(x) = \mathcal{N}_n \varphi_0(x) H_n(s(x)), \quad (17)$$

where $\mathcal{N}_n = (\sqrt{\pi} 2^n n!)^{-1/2}$. So the THO method is a particular case of the OP method, where the relevant polynomials are Hermite polynomials, the weight function is a Gaussian, and the local scale transformation is one that converts the ground state of the system in the ground state of a harmonic oscillator.

In the case of x values restricted to positive values, as in radial wave functions or semi-infinite potentials, it is more convenient to take only odd harmonic oscillator wave functions, for which the LST is given by

$$\int_0^x |\varphi_0(x')|^2 dx' = \int_0^s s'^2 |\phi_0^{HO}(s')|^2 ds', \quad (18)$$

and the THO basis is obtained by multiplying the ground state by Laguerre polynomials in the variable $s(x)^2$ [11]:

$$\phi_n^{THO'}(x) = \mathcal{N}_n' \varphi_0(x) L_n^{1/2}(s(x)^2), \quad (19)$$

where $\mathcal{N}_n' = [\Gamma(n+3/2)/n!]^{-1/2}$.

B. Trivial orthogonal polynomial method

In this method the local scale transformation is taken as the trivial transformation $s=x$. The ground state wave function in terms of s is just $\varphi_0(x)$. The weight function is

$$\omega(x) = |\varphi_0(x)|^2. \quad (20)$$

Orthogonal polynomials $P_n(x)$ in the interval $(-\infty, +\infty)$ with respect to this weight function can be found by a Gram-Schmidt procedure as sketched below. From these and the ground state wave function, the trivial orthogonal polynomial (TOP) basis wave functions are obtained as

$$\phi_n^{TOP}(x) = \mathcal{N}_n \varphi_0(x) P_n(x). \quad (21)$$

$P_n(x)$ can be written

$$P_n(x) = \sum_{k=0}^n C_{n,k} x^k. \quad (22)$$

The coefficients $C_{n,k}$ can be efficiently calculated taking $C_{n,n}=1$ and defining the moments

$$L_n = \int_{-\infty}^{\infty} dx \omega(x) x^n. \quad (23)$$

Orthogonality of $P_n(x)$ implies that

$$\sum_{k,k'} C_{n,k} C_{m,k'} L_{k+k'} = 0, \quad \forall m \neq n, \quad (24)$$

which allows us to calculate the coefficients of $P_n(x)$.

Summarizing, the trivial orthogonal polynomial method is a particular case of the OP method for which the local scale transformation is the identity $s=x$, the weight function of the polynomials is just the ground state density, and the orthogonal polynomials are calculated from knowledge of the moments of x in the ground state.

The TOP method has the property that the inclusion of just one state apart from the ground state is sufficient to give exactly the value of the total strength and the energy weighted sum rule of the operator $O(x)=x$ on the ground state. This is not surprising, because the second state in the TOP method is obtained by acting with the x operator on the ground state and orthogonalizing.

C. Natural orthogonal polynomial method

The THO and TOP methods are applicable to ground state wave functions derived from arbitrary Hamiltonians. Here we will consider two cases of analytic potentials for which there is a definite choice of natural variables in terms of which the wave functions acquire especially compact expressions [the natural orthogonal polynomial (NOP) method]. These cases are the Morse and Pöschl-Teller potentials.

1. Morse potential

The Morse potential [13] is

$$v(x) = D\{[1 - \exp(-x)]^2 - 1\}, \quad (25)$$

where $x = \alpha r$, with r the relative coordinate and α the inverse of the potential range, and D is the potential depth at the minimum ($x=0$). D can be written in terms of a parameter j [14], which is a positive real number, as

$$D = \frac{1}{2} \left(j + \frac{1}{2} \right)^2. \quad (26)$$

The normalized ground state wave function for the Morse potential characterized by the quantum number j is,

$$\begin{aligned} \phi_{j0}^M(x) &= \frac{1}{\sqrt{\Gamma(2j)}} (2j+1)^j \exp(-jx) \exp[-(j+1/2) \\ &\times \exp(-x)]. \end{aligned} \quad (27)$$

With this one can proceed with the formalism presented in the preceding section by choosing a LST $s(x)$. In this case the function $s(x)$ is chosen as the natural variable for the Morse potential

$$s = (2j+1) \exp(-x). \quad (28)$$

The variable s is defined between 0 and ∞ . Then, the normalized Morse ground state wave function as a function of s is written as

$$\phi_{j0}^M(s) = \frac{1}{\sqrt{\Gamma(2j)}} s^j \exp(-s/2). \quad (29)$$

Equations (3)–(5) define then the discrete basis associated with this transformation. The weight function is

$$\omega(s) = \frac{1}{\Gamma(2j)} s^{2j-1} \exp(-s), \quad (30)$$

and the discrete basis is related to the generalized Laguerre polynomials $L_n^{(2j-1)}(s)$,

$$\phi_{jn}^{NOP}(s) = N_{jn} L_n^{(2j-1)}(s) \phi_{j0}^M(s), \quad (31)$$

$$N_{jn} = \sqrt{\frac{n! \Gamma(2j)}{\Gamma(2j+n)}}.$$

It should be noticed that the Morse potential has a very simple expression in terms of the natural variable:

$$v(s) = \frac{1}{8} [s^2 - (4j+2)s]. \quad (32)$$

2. Pöschl-Teller potential

The Pöschl-Teller potential [15] is written as

$$v(x) = -D \frac{1}{\cosh^2(x)}, \quad (33)$$

where $-D$ is the value of the potential at its minimum. The variable $x = \alpha r$, where r is the relative coordinate and α is the inverse of the range of the potential. The depth of the potential D can be written as

$$D = \frac{1}{2} j(j+1), \quad (34)$$

in terms of a new parameter j [16] which is a positive real number. The normalized ground state wave function for the Pöschl-Teller (PT) potential characterized by the quantum number j is

$$\phi_{j0}^{PT}(x) = \sqrt{\frac{(2j-1)!!}{2^j(j-1)!}} \frac{1}{\cosh^j x}. \quad (35)$$

As in the case of the Morse potential, we present in this subsection the LST in which the function $s(x)$ is chosen as the natural variable for the Pöschl-Teller potential:

$$s = \tanh(x). \quad (36)$$

Then the normalized ground state wave function is written as

$$\phi_{j0}^{PT}(s) = \sqrt{\frac{(2j-1)!!}{2^j(j-1)!}} (1-s^2)^{j/2}. \quad (37)$$

Equations (3)–(5) define the discrete basis associated with this transformation. The weight function is

$$\omega(s) = \frac{(2j-1)!!}{2^j(j-1)!} (1-s^2)^{j-1}, \quad (38)$$

and the discrete basis is related to the Gegenbauer polynomials $C_n^{(j-1/2)}(s)$:

$$\phi_{jn}^{NOP}(s) = N_{jn} C_n^{(j-1/2)}(s) \phi_{j0}^{PT}(s), \quad (39)$$

$$N_{jn} = \sqrt{\frac{n!(n+j-1/2)[\Gamma(j-1/2)]^2}{\pi 2^{2-2j} \Gamma(2j+n-1)}} \sqrt{\frac{2^j(j-1)!}{(2j-1)!!}}.$$

Note that the potential can be written here also as a quadratic expression in terms of the natural variable:

$$v(s) = \frac{j(j+1)}{2} (s^2 - 1). \quad (40)$$

IV. APPLICATION TO MULTIBOUND POTENTIALS IN ONE DIMENSION

We have applied the formalism presented above to three cases of interest: the Morse potential, the Pöschl-Teller potential, and the semi-infinite square well. In each case we have used the THO, TOP, and NOP methods and have calculated the convergence of global observables that connect the ground state with the states in the continuum. In this section we present some of these results as an illustration.

A. Morse potential

We consider a Morse potential characterized by $j=4$, which has four bound states, and analyze the three methods discussed in the preceding section: THO, TOP, and NOP.

First the selected local scale transformation has to be computed: Eq. (16) for THO, $s=x$ for TOP, or Eq. (28) for NOP. Then the corresponding basis is constructed. In Fig. 1 we present the bases for THO, TOP, and NOP. It can be observed that the basis provided by NOP, due to the behavior of the corresponding LST, is concentrated close to the range of the potential, while THO and TOP allow a spreading over larger distances compared to the range of the ground state wave function. This would suggest that the NOP transformation is well suited for describing short range operators. On the other hand, the THO and TOP transformations would be more appropriated to describe long range operators.

Once the basis is obtained the Hamiltonian matrix is constructed by evaluating Eq. (11). Hamiltonian diagonalization in each basis provides us with eigenvalues and eigenfunctions. We plot in Fig. 2 the energies obtained for the three

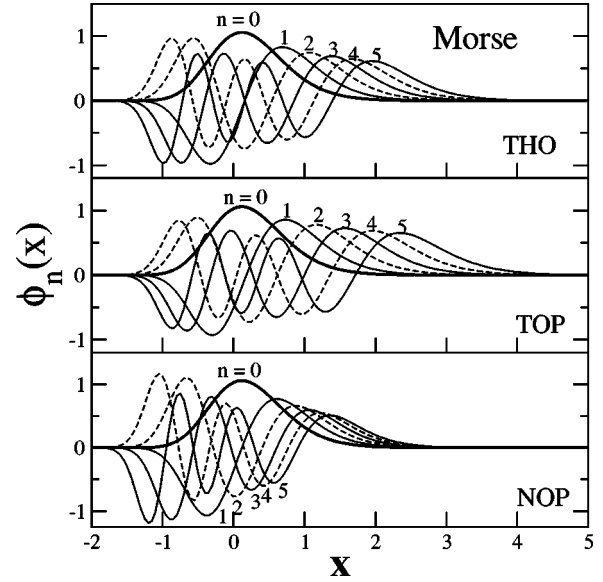


FIG. 1. $N=6$ basis for the Morse potential with $j=4$ in the THO, TOP, and NOP cases (x is dimensionless).

methods on increasing the dimension of the basis from $N=4$ to 12. The ground state energy lies always at its exact value $e_0 = -j^2/2 = -8$. The other three bound states move down in energy as the basis dimension is increased, and the convergence to the exact values is fast for THO and TOP and slower for NOP. In Table I the overlaps squared of the calculated $n=3$ state with the known least bound eigenfunction for the Morse potential are shown at the left. It can be seen that the THO and, especially, the TOP methods give appropriate descriptions of the least bound state. The NOP method converges very slowly.

We have investigated the convergence of the total strength, energy weighted sum rule, and polarizability for the

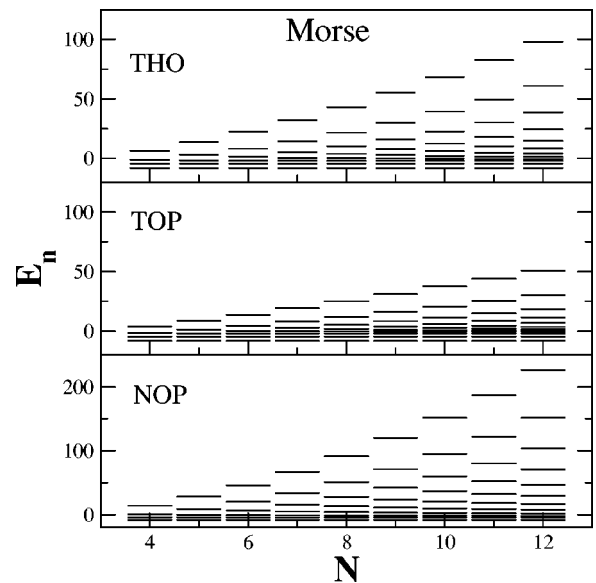


FIG. 2. Energy eigenvalues (dimensionless) for the Morse potential with $j=4$ in the THO, TOP, and NOP cases, as a function of the size of the basis.

TABLE I. Overlap squared of the calculated states with $n=3$ with the corresponding exact least bound state in the Morse, Pöschl-Teller, and SISW potentials as a function of the discrete basis dimension. All these potentials are taken to have four bound states (see text). Three cases are presented for the LST: THO, TOP, and NOP. N is the total number of basis states.

N	Morse			Pöschl-Teller			SISW	
	THO	TOP	NOP	THO	TOP	NOP	THO	TOP
6	0.202629	0.500192	0.000151944	0.819445	0.911	0.510256	0.254974	0.955693
8	0.508298	0.84243	0.0170537	0.927228	0.978336	0.624862	0.644374	0.997276
10	0.746842	0.964903	0.0562563	0.971845	0.995182	0.704354	0.930997	0.998823
12	0.884909	0.993699	0.10753	0.989412	0.998981	0.761336	0.985486	0.999810

operators x and $v(x)$ using the different discretization procedures as the dimension of the basis is increased. We find that the convergence is satisfactory in all cases. In Tables II and III we show the values obtained for $N=10$ for THO, TOP, and NOP compared to the exact values. For the long range operator x , the TOP method gives the exact result for the total strength and energy weighted sum rule, while for the short range operator $v(x)$, it is the NOP method that gives the exact values for these magnitudes. The THO method gives rapid convergence to the exact results in all cases. In anycase, the three methods give deviations that are less than 1 per thousand for the three observables calculated.

B. Pöschl-Teller potential

We have also performed calculations for a Pöschl-Teller potential with $j=4$ that has four bound states, two with positive parity and two with negative parity. In this case the local scale transformations for THO, TOP, and NOP are obtained from Eq. (16), $s=x$, and Eq. (36) respectively. All of them are odd functions of x . As in the preceding case we have studied the convergence of the calculated energies for the bound states to the exact values and the overlaps of the three lowest calculated excited states with the corresponding known bound eigenfunctions. In Table I the overlaps squared of the calculated $n=3$ state with the known least bound eigenfunction for the Pöschl-Teller potential are shown. In this case also, the convergence is faster in the THO and TOP methods, compared to the NOP method. Similarly to the Morse case presented above, we have computed the eigenvalues and the eigenfunctions of the Hamiltonian for each LST. The energy spectrum presents in this case a doublet structure. This fact reflects the alternating parity of the states.

Note that when the basis is increased by a state of a given parity, the eigenvalues and eigenstates of the opposite parity do not change.

With the eigenfunctions we have performed the convergence tests for the observables total strength, energy weighted sum rule, and polarizability. As for the Morse potential, convergence is faster in the TOP method for long range operators and in the NOP method for the short range operator, while the THO method is good in both cases. As shown in Tables II and III, the agreement of the calculation for $N=10$ in THO, TOP, and NOP methods with the exact values is better than 3 per thousand. As in the previous case, for the long range operator x , the TOP method gives the exact result for the total strength and energy weighted sum rule, while for the short range operator $v(x)$, it is the NOP method that gives the exact values for these magnitudes. The THO method gives rapid convergence to the exact results in all cases.

C. Semi-infinite square well in one dimension

As an additional example we develop here the formalism presented above for the semi-infinite square well (SISW) in one dimension (note that this is equivalent to solving the three-dimensional problem of a square well considering only $\ell=0$ states),

$$h = \begin{cases} \infty & \text{if } x \leq 0, \\ -v_0 & \text{if } 0 < x < a, \\ 0 & \text{if } x > a. \end{cases} \quad (41)$$

We choose the parameters $a=2$ and $v_0=18$, so that there are

TABLE II. Values of the total strength (S), energy weighted sum rule (E_w), and polarizability (P) for the operator x in a basis with 10 states ($N=10$) for Morse, Pöschl-Teller, and SISW Hamiltonians with four bound states each. Three cases are presented for the LST in each case: THO, TOP, and NOP. In the total strength (S) the diagonal contribution coming from the ground state has been removed.

$N=10$	$S(x,N)$			$E_w(x,N)$			$P(x,N)$		
	Morse	PT	SISW	Morse	PT	SISW	Morse	PT	SISW
THO	0.133137	0.141911	0.155092	0.5	0.5	0.496718	0.0366355	0.0404303	0.0493592
TOP	0.133137	0.141911	0.155241	0.5	0.5	0.5	0.0366355	0.0404303	0.0493675
NOP	0.133136	0.141911		0.500044	0.500016		0.0366236	0.040426	
Exact Value	0.133137	0.141911	0.155241	0.5	0.5	0.5	0.0366355	0.0404303	0.0493684

TABLE III. Same as Table II but for the short range operator $v(x)$.

$N=10$	$S(x,N)$			$E_w(x,N)$			$P(x,N)$		
	Morse	PT	SISW	Morse	PT	SISW	Morse	PT	SISW
THO	2.25	1.7957	1.10480	24.75	12.4313	32.4966	0.28125	0.274348	0.0579506
TOP	2.25	1.79518	0.942975	24.75	12.4013	22.4319	0.28125	0.274347	0.0560974
NOP	2.25	1.79574		24.75	12.432		0.281146	0.274247	
Exact value	2.25	1.79574	1.4872	24.75	12.432	∞	0.28125	0.274348	0.0582423

four bound states at energies $e_0 = -16.9504$, $e_1 = -13.8231$, $e_2 = -8.70546$, and $e_3 = -1.95092$. Defining $k_1 = \sqrt{2(v_0 + e_0)}$, $k_2 = \sqrt{-2e_0}$,

$$\phi_0^{SISW}(x) = \begin{cases} N_1 \sin(k_1 x) & \text{if } x \leq a, \\ N_2 \exp(-k_2 x) & \text{if } x > a, \end{cases} \quad (42)$$

where N_1 and N_2 are fixed by continuity at the boundary and normalization.

In this case, the THO method makes use only of even polynomials, as shown in Eq. (19). In Fig. 3 the basis functions are presented. The Hamiltonian matrix is constructed by evaluating Eq. (11). Hamiltonian diagonalization in the THO or TOP basis provides us with eigenvalues and eigenfunctions. We plot in Fig. 4 the energies obtained by increasing the dimension of the basis from $N=4$ to 12. In both cases the ground state energy lies at its exact value, $e_0 = -16.9504$. The other three bound states move down as the basis dimension is increased, and the convergence to the exact values is fast. The convergence of the overlaps of the $n=3$ calculated excited state with the corresponding known least bound eigenfunction for the semi-infinite square well potential is very fast for both THO and TOP cases, as shown in Table I. However, although both methods are very good, the TOP method is better for the purpose of reproducing the bound states.

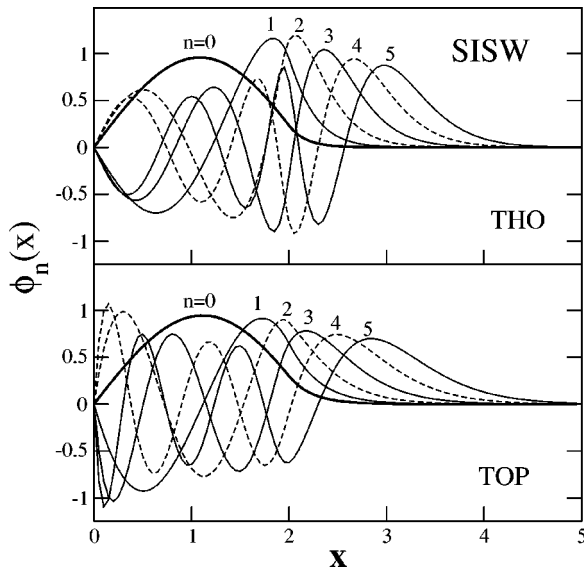


FIG. 3. $N=6$ basis for the SISW potential considered in the THO and TOP cases (x is dimensionless).

We have calculated for the THO and TOP the convergence of the total strength, energy weighted sum rule (EWSR), and polarizability for the operators x and $v(x)$ as the dimension of the basis is increased. It should be noticed that the square well potential has a sharp edge, and this produces the divergence of the EWSR. As a reflection of this, in our calculation the EWSR is larger and larger as the dimension of the basis is increased. In Tables II and III we show the calculated values for $N=10$ in the THO, TOP, and NOP methods compared with the exact values. For the long range operator x the exact results for the total strength and EWSR are obtained in the TOP case, and the convergence is very good in the THO case. For the short range operator $v(x)$ the convergence is rather poor for the total strength but the value of the polarizability is obtained within 2% in the $N=10$ calculation.

V. RELATION WITH THE TRUE CONTINUUM

We investigate the relation of the wave functions obtained in the OP methods that represent the continuum with the true continuum wave functions for the square well potential.

As the states $n=1,2,3$ reproduce the excited bound states accurately, the rest of the states, from $n=4$ onward, correspond to continuum states, with a very small admixture of excited bound states.

For the case of the semi-infinite square well the true continuum wave functions are known. However, a direct comparison of the OP wave functions with the continuum wave functions requires one to take care of the issue of normalization of the true continuum wave function. The true bound states $\psi_b(r)$ and the true continuum wave functions $\psi(k,r)$ have to satisfy closure:

$$\sum_b \psi_b(r) \psi_b(r') + \int dk \psi(k,r) \psi(k,r') = \delta(r-r'). \quad (43)$$

This implies that, for large distances, beyond the range of the potential, the continuum wave functions behave as

$$\psi(k,r) \rightarrow \sqrt{\frac{2}{\pi}} \sin(kr + \delta_k). \quad (44)$$

For the OP wave functions, the condition of closure becomes

$$\sum_{n=0}^{\infty} \phi_n(r) \phi_n(r') = \delta(r-r'). \quad (45)$$

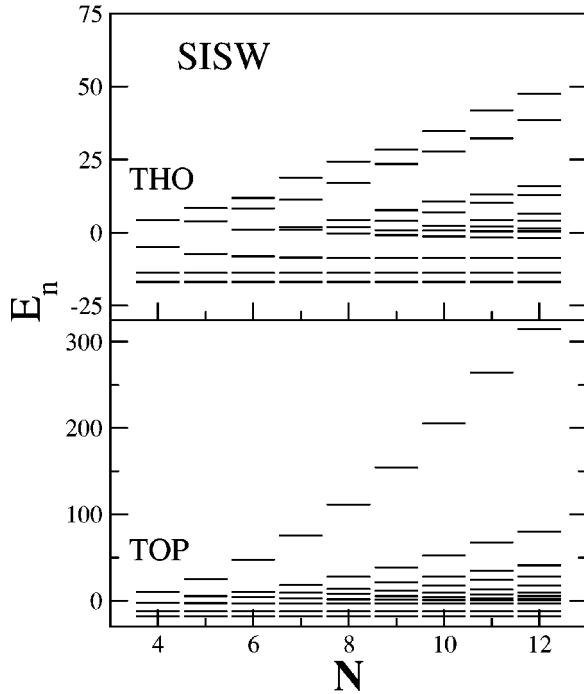


FIG. 4. Energy eigenvalues (dimensionless) for the SISW potential in the THO and TOP cases, as a function of the size of the basis.

When only a finite number of OP states are considered, the condition of closure will not be satisfied exactly, but one can have an arbitrarily accurate approximation. We can calculate the overlap between the eigenstates of the Hamiltonian in a finite OP basis with the true bound states, as well as with the true continuum states,

$$\langle N, i | b \rangle = \int dr \psi_i^N(r) \psi_b(r), \quad (46)$$

$$\langle N, i | k \rangle = \int dr \psi_i^N(r) \psi(k, r). \quad (47)$$

The condition of orthogonality of these overlap functions is

$$\sum_b \langle N, i | b \rangle \langle b | N, j \rangle + \int dk \langle N, i | k \rangle \langle k | N, j \rangle = \delta(i, j). \quad (48)$$

In addition, in order to perform a comparison we slice the continuum into bins in such a way that each bin is characterized by an interval of momentum (k_i^-, k_i^+) . The bin wave function is then obtained as a superposition of continuum wave functions within the bin

$$\Phi_i^{bin}(x) = \sqrt{\frac{2}{\pi(k_i^+ - k_i^-)}} \int_{k_i^-}^{k_i^+} dk \psi(k, x). \quad (49)$$

The interval of the bins $[k_i^-, k_i^+]$ is defined by the k values of the eigenstates obtained in the OP discretization. If we call $k_4, k_5, k_6, \dots$ the momentum of the OP eigenstates in the continuum (remember that for the cases considered we have

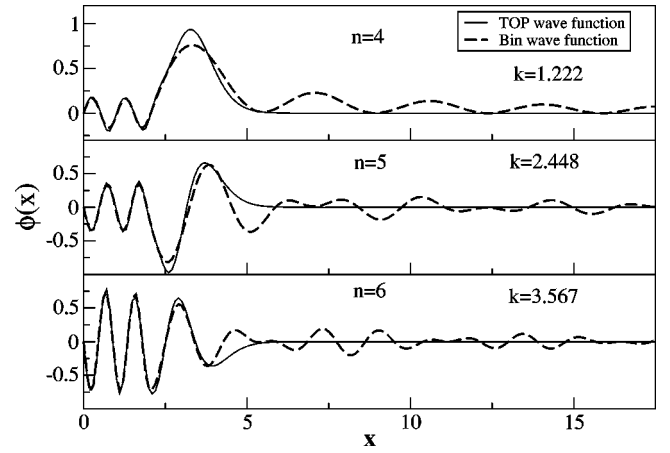


FIG. 5. Comparison of the first few continuum eigenstates of the SISW Hamiltonian in the TOP basis with the bin continuum wave functions constructed as a superposition of true continuum wave functions as explained in the text. The quantities plotted are dimensionless.

four bound states), the bins will be $[k_1^-, k_1^+] = [0, (k_5 + k_4)/2]$, $[k_2^-, k_2^+] = [(k_5 + k_4)/2, (k_6 + k_5)/2]$, $\dots$. We have approximated the integral (49) by a sum over 50 k -equidistant points inside the bin and present a comparison of the first few continuum bin functions with the wave functions obtained with the TOP method in Fig. 5 (similar results are obtained for the THO method). It can be seen that the TOP wave functions are in reasonably good agreement with the corresponding bin wave functions, especially at relatively small distances. This indicates that the OP method is closely related to the continuum discretized method as used for coupled channels calculations (CDCC). It should also be noticed that the OP wave functions do not display the long range oscillatory behavior that is characteristic of the bin wave functions. This can be an advantage when using OP wave functions as an alternative to bin wave functions in CDCC calculations.

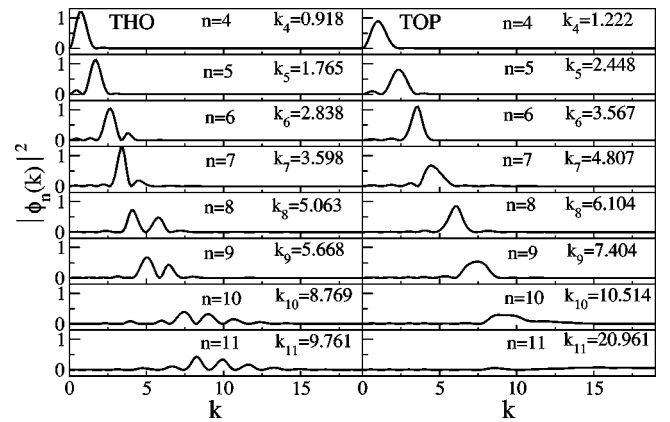


FIG. 6. Expansion of the THO (left hand side panels) and TOP (right hand side panels) continuum ($n=4$ to $n=11$) wave functions squared in terms of the asymptotic momentum k for the SISW potential considering a basis with $N=12$ states. The quantities plotted are dimensionless.

In Fig. 6 we represent, for the case of a base with $N=12$ states, the square of the OP wave functions that represent the continuum as a function of the asymptotic momentum of the states. The left panels correspond to the THO method while the right panels are for the TOP method. It should be noticed that the OP states correspond to a superposition of true continuum states which is extended to a relatively narrow range of momenta. This range is reduced as the size of the OP basis is increased, so that, in the limit of large N , the OP states should coincide with the true continuum states. In the TOP case, the wave functions correspond to a relatively narrow range of momentum values, except for the state with the higher energies. Thus, the TOP wave functions can be interpreted as localized wave packets of momentum states. In the THO case, the wave functions of low excitation energy do correspond to a narrow range of momenta. However, for the higher energies, the THO wave functions display a structure in momentum space that indicates that they are not just wave packets.

VI. SUMMARY AND CONCLUSIONS

We have formulated a general orthogonal polynomial method to discretize the continuum in one-dimensional problems. The method generates a complete discrete basis of normalizable states. These are obtained by multiplying the ground state of the system by a family of orthogonal polynomials on a suitable variable s , which is obtained from a local scale transformation $s(x)$ on the physical variable x . The local scale transformation, along with the ground state of the system, determines the weight function for the family of orthogonal polynomials.

We obtain the transformed harmonic oscillator method as a particular case of the OP method, for which the relevant polynomials are Hermite. Also, we derive the trivial orthogonal polynomial method by taking the local scale transformation as the identity $s(x)=x$. For special potentials, such as

the Morse and Pöschl-Teller potentials, a natural orthogonal polynomial method can be used, using the natural variables of these potentials to define the local scale transformations. The relevant polynomials are Laguerre in the Morse case and Gegenbauer in the Pöschl-Teller case.

The different OP methods are compared by checking the convergence of relevant sum rules of long and short range operators which couple the ground state to the other bound states and the continuum states. It is found that the TOP method is optimal for long range operators, while the NOP method is more adequate for short range operators. The THO method appears as a good compromise option which works well in both cases.

We have also investigated the description of excited bound states in the different variants of the OP method. We find that the THO and TOP methods give fast convergence for both energies and wave functions of bound states, while for the NOP method the convergence is slower.

For the case of the semi-infinite square well potential, the true continuum states and the states obtained from continuum discretization by the TOP and THO methods are compared. The radial behavior of the THO and TOP wave functions compares reasonably well with the radial behavior of bins built from the continuum wave functions. It is found that the lower states obtained from continuum discretization in a finite basis can be understood as wave packets of the true continuum states, the width of which decrease as the size of the basis is made larger. For the states of higher excitation energy, the wave packet interpretation is still adequate for the TOP method, but not so for the THO states.

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