Simple approach for the bound-state energy spectrum of the generalized exponential-cosine Coulomb potential

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Based on the series expansion formalism, a relatively simple approach is proposed to solve the eigenvalues problems with partially screened and screened exponential-cosine Coulomb potentials. This approach is used to derive solutions to the Schrödinger equation with the two forms of potentials. The eigenenergies are explicitly deduced from solving the obtained corresponding polynomial equations. For illustration, high accuracy results have been obtained in the entire range of parameter values of these potential forms, with no constraints or adjustable constants. The present approach compares well, with existing methods, the results of which are precisely recovered as particular cases and does allow solutions to eigenvalues problems with any combination of potential parameters.

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I. INTRODUCTION

It is well known that the generalized exponential-cosine screened Coulomb (ECSC) potential $V(r) = \exp(-\mu r)\cos(\lambda r)/r$ belongs to a wide class of model potentials used in different areas of physics. Theoretical investigations of the ECSC potential have been performed through various numerical and analytical approaches for the determination of the energy eigenvalues and the corresponding wave functions [1–8]. The particular case $\mu = \lambda$ of this type of potential has been treated by perturbation theory with λ as perturbation parameter along with a constraint on the scaling parameter [1–4]. The accuracy obtained is up to the first five decimals. For the same case ($\mu = \lambda$), the large-N expansion technique was applied to obtain the bound-state energy spectrum [6,7]. A power series-Hill determinant method has been developed by Killingbeck [7] to calculate the energy eigenvalues for some particular values of μ and λ. An adjustable constant and a scaling factor have been introduced. A trial energy value is required in the calculations. Recently, Ixaru *et al.* [8] have presented a procedure for numerical solution of the eigenvalues problems with the distorted Coulomb potential. In that work, the partially screening exponential-cosine (PSEC) potential is assumed to describe two regions corresponding to two different electric charges, which are located around the origin and at the asymtotic limit, respectively. In this procedure the knowledge of the behavior of $V(r)$ is not required. However, it is well known that some physical problems are mainly concerned by the short and intermediate distances (e.g., potential models for hadron physics). Moreover, the success of direct numerical integration methods depends on the quality of initial guesses of the trial eigenvalues and boundary conditions.

In the present work, a simple approach is proposed to determine highly accurate eigenvalues of the generalized exponential-cosine Coulomb potentials. The series expansion formalism is used to derive analytical solutions to the Schrö-dinger equation for two forms of the considered potential. Once these solutions have been obtained, the corresponding polynomial equations will allow the determination of the sequences of energy levels for a given set of potential parameters, and fixed angular momentum l, without resorting to extensive numerical calculations. Thus, the uncertainties related to the use of approximate methods and the singularity problems are avoided. The proposed approach, which requires neither adjustable constants nor starting trial energy value, can be extended to potentials of the same form occurring in nuclear physics and condensed matter.

After the Introduction, in Sec. II, recursion relations are derived in order to construct solutions to the Schrödinger equation with two forms of the ECSC potential: the generalized exponential-cosine screened Coulomb potential and the partially screening exponential-cosine Coulomb potential. In Sec. III, the present work is illustrated by calculations of the eigenenergies in a whole range of parameters values of the considered potential forms. Some numerical results are presented and compared with previous computations that were performed by other methods.

II. SERIES SOLUTION FOR THE POTENTIALS

A. The generalized exponential-cosine screened Coulomb potential

The radial part of the time-independent Schrödinger equation with ECSC potential and centrifugal term can be written in the following form (atomic units are used throughout):

$$\psi''(\rho) + \left[-\varepsilon^2 - \frac{l(l+1)}{\rho^2} + 2\beta \frac{e^{-\rho}\cos(\kappa\rho)}{\rho} \right] \psi(\rho) = 0, \tag{1}$$

where $\varepsilon = \sqrt{-2E}/\mu$, $\kappa = \lambda/\mu$, and $\beta = a/\mu$, E being the eigenvalue to be looked for (only the bound states are considered). Here μ and λ are the usual screening parameters of

TABLE I. Energy eigenvalues $(-E$, in a.u.), for $l=0$ and different values of screening parameters (μ,λ) of ECSC potential. The number of terms used is $N=14$. Only six decimals are quoted here. The underlined values, located on the first diagonal of the table, correspond to the results obtained for the particular case $\mu=\lambda$ by other methods [1–7].

$\mu\backslash\lambda$	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09	0.1	0.2
0.01	<u>0.490001</u>	0.480224	0.470591	0.461100	0.451748	0.442533	0.433453	0.424504	0.415686	0.406996	0.326740
0.02	0.489781	<u>0.480008</u>	0.470379	0.460892	0.451544	0.442333	0.433256	0.424311	0.415496	0.406810	0.326585
0.03	0.489413	0.479648	<u>0.470026</u>	0.460546	0.451204	0.441999	0.432928	0.423989	0.415180	0.406499	0.326326
0.04	0.488900	0.479144	0.469532	<u>0.460061</u>	0.450728	0.441532	0.432470	0.423539	0.414738	0.406065	0.325964
0.05	0.488240	0.478497	0.468898	0.459438	<u>0.450117</u>	0.440932	0.431881	0.422961	0.414170	0.405507	0.325498
0.06	0.487436	0.477708	0.468123	0.458679	0.449372	<u>0.440201</u>	0.431162	0.422255	0.413477	0.404827	0.324929
0.07	0.486487	0.476778	0.467210	0.457783	0.448492	0.439337	<u>0.430315</u>	0.421423	0.412660	0.404023	0.324256
0.08	0.485395	0.475706	0.466159	0.456751	0.447480	0.438343	0.429338	<u>0.420464</u>	0.411718	0.403098	0.323480
0.09	0.484160	0.474495	0.464971	0.455585	0.446335	0.437218	0.428234	0.419380	<u>0.410653</u>	0.402052	0.322600
0.1	0.482785	0.473145	0.463646	0.454284	0.445058	0.435965	0.427003	0.418170	0.409465	<u>0.400885</u>	0.321616
0.2	0.461597	0.452339	0.443211	0.434211	0.425337	0.416588	0.407962	0.399457	0.391071	0.382804	<u>0.306375</u>

the potential and a is a constant. The ECSC potential in Eq. (1) can be represented as an infinite series of the form

$$V(\rho)=2\beta\sum_{p=0}^{\infty}\sum_{q=0}^{p} g_{p-2q}h_q\rho^{p-1}, \qquad (2)$$

where g and h are the series expansion coefficients of the exponential and cosine functions, respectively. The objective now is to construct an analytical solution of Eq. (1) with the potential form (2). This solution is sought in the form

$$\psi(\rho)=\rho^{s}e^{-\varepsilon\rho}\phi(\rho), \qquad (3)$$

where s is determined in such a way that the solution goes to zero at the origin. Substituting Eqs. (3) and (2) into Eq. (1), we obtain

$$[s(s-1)-l(l+1)]\phi+(2s\phi'-2\varepsilon s\phi)\rho+(\phi''-2\varepsilon\phi')\rho^2$$

$$+2\beta\phi\sum_{p=0}^{\infty}\sum_{q=0}^{p} g_{p-2q}h_q\rho^{p+1}=0, \qquad (4)$$

where the variable ρ of the function ϕ is omitted for simplicity. The function $\phi(\rho)$ can be represented by a series expansion whose coefficients will be determined by the standard procedure (see, e.g., Ref. [9])

$$\phi(\rho)=\sum_{k=0}^{\infty} \alpha_k\rho^k. \qquad (5)$$

The expansion coefficients α_k and the basis functions $\phi(\rho)$ are real. Substituting the expansion (5) into Eq. (4) and equating the terms of successive powers of ρ to zero, we obtain the following recurrence relation for the coefficients α_n,

$$\alpha_n=\frac{(n+l)\varepsilon\alpha_{n-1}-\beta\sum_{p=0}^{n-1}\sum_{q=0}^{p} g_{p-2q}h_q\alpha_{n-1-q}}{n\left(l+\dfrac{n+1}{2}\right)}, \quad n\geqslant 1. \qquad (6)$$

So far, we have not introduced any constraint or adjustable constant in these calculations. Finally an analytical solution to the Schrödinger equation with the generalized exponential-cosine screened Coulomb potential is obtained

$$\psi(\rho)=\rho^{l+1}e^{-\varepsilon\rho}\left(\alpha_0+\sum_{n=1}^{\infty} \alpha_n\rho^n\right), \quad \alpha_0\neq 0. \qquad (7)$$

The solution $\psi(\rho)$ is function of the angular momentum l, the bound-state eigenvalue E (i.e., ε, to be calculated) and the two screening parameters μ and λ.

TABLE II. Energy eigenvalues (a.u.) versus the number N of terms of the polynomial equation for the ECSC potential. The second column corresponds to the eigenvalue $(E=-0.490\,001)$ displayed in Table I for $(\mu,\lambda)=(0.01,0.01)$. The values in the last line are the results with $N=50$ of Ref. [7].

N	$(0.01,0.01)l=0$	$(0.05,0)l=0$	$(0.05,0)l=1$
8	-0.490000987578414	-0.45181642236646	-0.08046402435766
10	-0.490000987578416	-0.45181642843260	-0.08069564787830
13	-0.490000987578417	-0.45181642852304	-0.08073227047680
14	-0.490000987578417	-0.45181642852448	-0.08073875332339
16	-0.490000987578418	-0.45181642852449	-0.08074036232384
50		-0.45181643	-0.08074039

TABLE III. Energy convergence (a.u.) versus the number of terms N of the polynomial equation and the value of the variable ρ for ECSC potential with $\mu=0.05$, $\lambda=0$ and $l=0$. In the last column are displayed the results of the power series–Hill determinant method [7].

$\rho\backslash N$	8	10	14	18	50
5	-0.4518164223	-0.4518164284	-0.4518164285	-0.4518164297	
10	-0.4518164284	-0.4518164284	-0.4518164285	-0.4518164298	-0.45181562
15	-0.4518164284	-0.4518164285	-0.4518164285	-0.4518164298	-0.45181643
20	-0.4518164284	-0.4518164285	-0.4518164285	-0.4518164298	-0.45181643
10^{20}	-0.4518164284	-0.4518164285	-0.4518164286	-0.4518164298	-0.45181643

B. The partially screening exponential-cosine Coulomb potential

The recurrence relation (6) and the constructed solution (7) correspond to the well known form of the ECSC potential used in Refs. [1–7]. In order to test the reliability of the proposed approach, it is of interest to consider also the partially screening exponential-cosine Coulomb potential used by Ixaru *et al.* [8]. This is one more motivation for the present work to make comparison with the most recent available numerical results. The PSEC potential is written in the following form (see Eq. (5.3) in Ref. [8]):

$$V(r)=-2Z_0V(r,\mu,\lambda)-2Z_{as}\left(\frac{1}{r}-V(r,\mu,\lambda)\right), \quad (8)$$

where Z_0 and Z_{as} are the charges corresponding to two assumed regions of the potential, for small and large distances r, respectively. By analogy with the form (2), the potential (8) can be represented in the following expansion:

$$V(\rho)=2\eta\left(b\sum_{p=0}^{\infty}\sum_{q=0}^{p}g_{p-2q}h_q\rho^{p-1}-\frac{1}{\rho}\right), \quad (9)$$

where $\eta=Z_{as}/\mu$ and $b=(Z_{as}-Z_0)/Z_{as}$. The coefficients g and h are defined in Eq. (2). The procedure developed above is applied to solve the corresponding equation with Eq. (9). For the sake of brevity, we omit the intermediate steps of

calculations and give only the final expression of α_n obtained for the PSEC Coulomb potential

$$\alpha_n=\frac{[(n+l)\varepsilon-\eta]\alpha_{n-1}+b\,\eta\sum_{p=0}^{n-1}\sum_{q=0}^{p}g_{p-2q}h_q\alpha_{n-1-q}}{n\left(l+\frac{n+1}{2}\right)},$$

$$n\geqslant 1. \quad (10)$$

The constructed solution is of the same form as Eq. (7), but with α_n derived in Eq. (10).

The wave function $\psi(\rho)$ and considered potentials strongly converge as $\rho\to\infty$ (ρ very large). The series over n in Eq. (7) are infinite but converge very rapidly. To avoid the drawbacks of the existing methods, presented in the introduction, it will be adopted in the present work, an approach based on the fact that, for large values of ρ and a given set of parameters that describe the considered potential, the series $\psi(\rho)$ in Eq. (7) can be considered as a nth degree polynomial equation in ε. In general, the problems that arise when one uses the power series expansion formalism are related to the determination of corresponding coefficients. In the present approach, these problems are avoided due to the recursive procedure derived for the successive evaluation of the coefficients α_n. Knowing that for a polynomial of degree

TABLE IV. Energy eigenvalues (a.u.) for $l=0$ and different values of the screening parameters (μ,λ) of the PSEC Coulomb potential. The noted down out at the bottom of the table values correspond to the results of Ref. [8] obtained for the particular case $\mu=\lambda=0.025$ (all quoted figures are kept).

$\mu\backslash\lambda$	0.023	0.024	0.025	0.026
0.024	-2497.648069565322	-2497.648000541650	-2497.647928580743	-2497.647853682713
	-662.648283005093	-622.648007571868	-622.647720419181	-622.647421545352
	-275.426432264287	-275.425815023098	-275.425171510940	-275.424501736108
0.025	-2497.550141591035	-2497.550072570069	-2497.550000612079[a]	-2497.549925717022
	-622.550571065078	-622.550295671433	-622.550008558031[b]	-622.549709726477
	-275.329080239292	-275.328463176982	-275.327819865708[c]	-275.327150293829
0.026	-2497.452216553854	-2497.452147535665	-2497.452075580554	2497.452000688449
	-622.452870845412	-622.452595489654	-622.452308416614	-622.542009627196
	-275.231754460659	-275.231137592236	-275.230494475763	-275.229825105659

[a] -2497.5500006120.
[b] -622.550008557.
[c] -275.327819864.

n there are always n (not necessary distinct) roots. In the present work the polynomial equation is solved by using a computational procedure based on the well-established Jenkins-Traub method [10] which converges very rapidly. The process of finding the successive roots of the polynomial equation, i.e., the eigenvalues, can be achieved by two possible ways. The first one gives n isolated roots while the second provides a product of first-degree and second-degree polynomials (this is in accordance with the fundamental properties of the polynomial algebra). The same expected roots are obtained in both cases with the same number of significant digits. This procedure permits, in a simple way, a straightforward determination of the energy levels without introducing any starting value of E or bracketed root.

III. COMPUTATIONAL RESULTS

Calculations have been carried out with the generalized ECSC potential for fixed values of l and screening parameters (μ,λ) varying from 0.01 to 0.2. The energy eigenvalues obtained for $l=0$ are displayed in Table I where only 6 decimals are shown. The underlined values, located on the first diagonal of this table, correspond to the particular case $\mu=\lambda$ which was treated by other methods in Refs. [1–7]. High accuracy results, up to sixteen significant figures, have been obtained with a relatively low number of terms ($N=14$) of the polynomial equation. To illustrate this precision with more digits, in Table II some specific results are presented for the case $\mu=\lambda=0.01$ ($E=-0.490\,001$) shown in Table I with only six digits. The case $\mu=0.05$ and $\lambda=0$ is not shown in this table. The results obtained in the framework of the Hill-determinant method (see the last line of Table II) require a number ranging from 20 to 50 terms [7]. On the other hand, we can notice from Table II, that the accuracy increases with increasing of number of terms, i.e., the fact of adding terms provides eigenvalues with more and more precision. This is very convenient in practical calculations since this procedure allows, in principle, the required accuracy to be reached. This process is analogous to the well known root-polishing technique of the numerical analysis [10]. The process of computation does not require any convergence acceleration procedure. Table III shows the energy convergence with respect to the number of terms considered in the polynomial equation and the values of the variable ρ for $l=0$. In the last column of this table the results obtained in the framework of the Hill-determinant method by using 50 terms are listed [7]. In the present approach the first ten significant figures are reached by using five terms only. From mathematical point of view, l does not have to be integer. The eigenvalues obtained for noninteger values of l are not shown in this paper. To verify the efficiency of the proposed approach, calculations have been performed for the partially screening exponential-cosine Coulomb potential (8) with screening parameters (μ,λ) varying from 0.023 up to 0.026, for $l=0,5$ and 10. Some results (for $l=0$) are presented in Table IV with about sixteen significant figures. Comparison is made with the most recent calculations for the particular case $\mu=\lambda=0.025$ [8].

In summary, highly accurate eigenvalues for two forms of the generalized exponential-cosine Coulomb potential can be obtained by a relatively simple approach, based on the series expansion formalism combined with solving of polynomial equations. The procedure of calculation, which can be applied to other potentials of similar form, permits, in a simple way, a straightforward determination of the energy eigenvalues without introducing any adjustable parameter or constraint. Singularity problems are avoided. All results previously obtained by other methods are reproduced here, as particular cases, with high accuracy. Predictions can be made for different combinations of potential parameters. The advantages of the proposed approach are speed, stability, and accuracy.

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