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Jost-function approach to quantum defect theory

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We present an approach to the quantum-defect theory theory using the Jost functions and Jost solutions as the main building blocks. An attractive feature of this approach is that it allows us to avoid use of the explicit form of the solutions of the radial Schrödinger equation for the Coulomb problem. We obtain a concise representation of the Jost function for the superposition of the Coulomb and short-range potentials, which distinctly separates terms analytic in k^2 and terms singular at $k = 0$. This representation can be used to design simple and efficient procedures allowing us to determine scattering phase shifts from the information about the bound states.

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I. INTRODUCTION

Quantum-defect theory (QDT) is a well-known method allowing us to describe a variety of atomic phenomena, such as photoionization or electron-ion scattering in terms of just a few parameters. The values of the parameters can be inferred either from the experimental data or from a theoretical calculation. These parameters, moreover, can be chosen to be slowly varying functions of energy in the reaction threshold region, which means that determining a set of the QDT parameters at a fixed energy, one obtains a description of the phenomena which may exhibit marked energy dependence, such as photoionization or autoionization profiles.

The QDT is based essentially on the properties of the radial wave functions describing electron motion in the Coulomb field. The foundation of the method was, therefore, laid out in 1928 [1] shortly after the advent of the quantum mechanics. The QDT has been subsequently elaborated by many workers. A (necessarily incomplete) list of the theoretical developments and applications of the QDT includes generalization to the multichannel case [2,3] and QDT description of various atomic [4–7] or molecular [8] processes. A relativistic version of QDT has been developed [9]. A detailed description of the history of the subject written by the founders of the QDT can be found in the review works [10,11].

The work done by these authors (and many others whom we can not cite for the lack of space) demonstrated great practical utility and versatility of the QDT method. It may not be an easy task to find a problem in atomic or molecular physics to which QDT has not been applied with success. Yet, occasionally, the subject is revisited. Thus, the work [12] reported a rigorous study of the character of the singularity of the S matrix at the threshold point $E = 0$ employing careful analysis of the regular and irregular Coulomb solutions. Such a study, we believe, is highly desirable. Indeed, in earlier works, the numerous practical implementations of QED were the priority, and mathematical rigor was of only secondary importance. For example, somewhat loose terms such as "almost analytical function" can be found in many papers and textbooks to describe the often encountered in QDT situation, when a function under study is a sum of a truly analytic (i.e., represented by a series convergent near the threshold point $E = 0$) function, and a function exponentially decreasing in some region of the complex k plane. Adding such an exponentially decreasing function to a truly analytic function changes completely the nature of the series used to represent the function near $E = 0$. A convergent series representing the function in a circle around the point $E = 0$ may become an asymptotic one, and asymptotic series generally can represent a given function only in some sector of a circle. Not taking proper account of this fact may lead to erroneous results as was demonstrated in [12]. Aside from the purely academic interest in determining the true nature of the singular point arising in QDT expressions, its proper description is important, therefore, from the purely pragmatic point of view. Having such a description at our disposal, we may devise reliable numerical schemes, in particular, the schemes for the extrapolation across the threshold point $E = 0$, which constitutes the main goal of QDT.

We should note also, and that is another motive of our undertaking this study, that in developing the QDT, emphasis is usually put on the various explicit forms of the solutions of the Coulomb-Schrödinger equation. Such an approach, we believe, may obscure to some extent the physical content of the theory which can not depend on the particular choice of the Coulomb solutions.

The theoretical exposition of QDT method can, we believe, be developed in a more concise and illuminating way. Following, we present an approach to the QDT theory based on the use of the Jost functions [13,14]. It is known that description of scattering based on the Jost functions can be used to describe near-threshold phenomena (such as zero-energy resonances) in a concise and economic way [15].

We are trying in what follows to achieve the same goal providing a description of the QDT method based on the Jost functions.

II. THEORY AND RESULTS

We shall recapitulate very briefly some well-known facts from the scattering theory on which the derivation presented

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below will rely. We consider the single-channel case and spherically symmetric potential, so that after separating radial and angular variables the radial Schrödinger equation for a given angular momentum l can be written as

$$-\frac{1}{2}\frac{d^2\phi}{dr^2}+\left(V(r)+\frac{\lambda^2-\frac{1}{4}}{2r^2}\right)\phi=\frac{k^2}{2}\phi, \qquad (1)$$

where the potential $V(r)=-\frac{1}{r}+V_s(r)$ is assumed to be a superposition of the Coulomb potential and a short-range potential $V_s(r)$ vanishing beyond certain $r=r_0$, $\lambda=l+\frac{1}{2}$.

Two Jost functions $f^+(\lambda,k)$ and $f^-(\lambda,k)$ can be introduced as usual [16], using solutions $f^+_\lambda(k,r)$ and $f^-_\lambda(k,r)$ (the Jost solutions) of Eq. (1) with boundary conditions $\lim_{r\to\infty} e^{-i(ikr+\frac{\ln 2kr}{k})} f^+_\lambda(k,r)=1$, and $\lim_{r\to\infty} e^{i(ikr+\frac{\ln 2kr}{k})} f^-_\lambda(k,r)=1$. Regular solution $\phi_\lambda(k^2,r)$ of Eq. (1) which will be convenient to us to normalize by the boundary condition $\Gamma(\lambda+\frac{1}{2})\lim_{r\to 0}\phi_\lambda(k^2,r)/r^{\lambda+\frac{1}{2}}=1$ can then be expressed using the Jost functions (this is in fact the definition of the Jost functions) as

$$\phi_\lambda(k^2,r)=\frac{1}{2ik}[f^-(\lambda,k)f^+_\lambda(k,r)-f^+(\lambda,k)f^-_\lambda(k,r)]. \qquad (2)$$

By the well-known Poincare theorem, solution (2) is an analytic (in fact entire) function of k^2. Functions $f^+(\lambda,k)$ and $f^-(\lambda,k)$ are regular and analytic in the upper and lower half planes of the complex plane k, respectively. In the region $\mathrm{Im}k>0$, function $f^+(\lambda,k)$ has a sequence of pure imaginary zeros $k_n=i\kappa_n$, where $\kappa_n=1/\sqrt{-2E_n}$, and E_n are the energies of the bound states with a given angular momentum l which our system may possess. These are the only zeros of $f^+(\lambda,k)$ in the upper half plane. On the real axis and for $k>0$, a relation $\delta_l=-\arg f^+(\lambda,k)$ holds, where δ_l is the scattering phase shift and $\arg f^+(\lambda,k)$ is the argument of the Jost function. The Jost function thus contains information about both energy levels of a system and the scattering phase shifts. Function $f^-(\lambda,k)$ possesses similar properties in the lower half of the k-complex plane.

Bound states and the scattering phase shifts being the two main ingredients of the QDT theory, Jost functions can provide us a means of the concise formulation of the theory. This can be done as follows. Consider first the pure Coulomb case, when short-range interaction in Eq. (1) is absent.

A. Coulomb case

The explicit form of the Jost functions is given in this case by [16] (for the sake of convenience we adopt a slightly different normalization)

$$f^\pm(\lambda,k)=\frac{(2k)^{-\lambda-\frac{1}{2}}e^{-\frac{\pi}{2k}}e^{\pm i\frac{\pi}{2}(\lambda-\frac{1}{2})}}{\Gamma\left(\lambda+\frac{1}{2}\mp\frac{i}{k}\right)}. \qquad (3)$$

We shall need below another solution of Eq. (1) for the Coulomb potential which would be an analytic function of k^2. It is known [16] that solution (2) can be continued analytically to the λ complex plane with excluded half-integer points on the negative real axis $\lambda=-\frac{1}{2},-\frac{3}{2}\ldots$.

By the Poincare theorem again, $f^+_\lambda(k,r)$ and $f^+_\lambda(k,r)$ being solutions of a differential equation depending analytically on a parameter, and satisfying boundary conditions not containing this parameter, are analytic functions of λ. Moreover, since parameter λ enters Eq. (1), only via λ^2 we can conclude that $f^+_\lambda(k,r)$ and $f^+_\lambda(k,r)$ are even analytic functions of λ, so that $f^\pm_\lambda(k,r)=f^\pm_{-\lambda}(k,r)$. Since analytic continuation in variable λ preserves analyticity in k^2, we may conclude that for $\lambda\neq\frac{1}{2},\frac{3}{2}\ldots$ the function

$$\phi_{1\lambda}(k^2,r)=\frac{1}{2ik}[f^-(-\lambda,k)f^+_\lambda(k,r)-f^+(-\lambda,k)f^-_\lambda(k,r)] \qquad (4)$$

will also be a solution of Eq. (1) analytic in k^2.

One can see from Eqs. (2), (3), and (4) that solutions ϕ_λ and $\phi_{1\lambda}$ become linearly dependent for the physically important case of λ belonging to the set C of the half-integers $\lambda_c=\frac{1}{2},\frac{3}{2}\ldots$, which corresponds to the integer values of angular momentum. Indeed, for these λ's the ratios of the coefficients with the functions $f^+_\lambda(k,r)$ and $f^-_\lambda(k,r)$ in Eqs. (2) and (4),

$$A^+(\lambda_c,k)=f^+(-\lambda_c,k)/f^+(\lambda_c,k) \qquad (5)$$

and

$$A^-(\lambda_c,k)=f^-(-\lambda_c,k)/f^-(\lambda_c,k) \qquad (6)$$

are equal, as can be easily seen from Eq. (3). It is easy to see from Eq. (3) also that $A(\lambda_c,k)=A^-(\lambda_c,k)=A^+(\lambda_c,k)$ is a polynomial in k^2.

For λ belonging to the set C of positive half-integers, we may define solution ϕ_2 analytic in k^2 by means of a limiting procedure

$$\phi_{2\lambda_c}(k^2,r)=\lim_{\lambda\to\lambda_c}\frac{A(\lambda_c)\phi_\lambda-\phi_{1\lambda}}{\lambda-\lambda_c}. \qquad (7)$$

This limit can be computed if we express in Eq. (7) $\phi_{1\lambda}$ in terms of ϕ_λ and $f^+_\lambda(k,r)$ using Eqs. (2) and (4) with the following result:

$$\phi_{2\lambda_c}(k^2,r)=-\phi_{\lambda_c}(k,r)\frac{\partial A^+(\lambda,k)}{\partial\lambda}\Big|_{\lambda=\lambda_c}+\alpha(\lambda_c,k)f^+_{\lambda_c}(k,r). \qquad (8)$$

The coefficient $\alpha(\lambda_c,k)$ in this equation can easily be expressed in terms of the Jost functions, but we shall not need its exact form below.

Having at our disposal analytic solutions given by Eqs. (2) and (8), we can find the Jost functions for the general case of the superposition of the Coulomb and short-range interactions in Eq. (1) as described in the following.

B. Superposition of the Coulomb and short-range interactions

From now on, we consider only the case of the positive half-integer values $\lambda=\lambda_c=l+\frac{1}{2}$ corresponding to the integer values of angular momentum l in Eq. (1). In the outer region, where short-range interaction vanishes, the regular solution $F_{\lambda_c}(k^2,r)$ of Eq. (1), analytic in k^2, can be represented as a combination of the Coulomb solutions we have defined above:

$$F_{\lambda_c}(k^2,r)=B(k^2)\phi_{\lambda_c}(k^2,r)+C(k^2)\phi_{2\lambda_c}(k^2,r), \qquad (9)$$

where $B(k^2)$ and $C(k^2)$ are some analytic functions of k^2.

Expressing Coulomb solutions by means of Eqs. (2) and (8) as combinations of the solutions $f^+_\lambda(k,r)$ and $f^-_\lambda(k,r)$, one can easily find that coefficient with $f^-_\lambda(k,r)$ in the

Eq. (9) will be given by the expression $B(k^2)f^+(\lambda_c,k) + C(k^2)f^+(\lambda_c,k)\frac{\partial A^+(\lambda,k)}{\partial\lambda}$, where the derivative is to be computed at the point $\lambda = \lambda_c$ corresponding to the physical integer value of the angular momentum. In the outer region, where Eq. (9) is valid, solutions $f_\lambda^+(k,r)$ and $f_\lambda^-(k,r)$ are the same both for the case of the pure Coulomb and for the superposition of the Coulomb and short-range interactions (they satisfy the same differential equation in the outer region and identical asymptotic boundary conditions). From the definition of the Jost functions in Eq. (2) and the discussion above, we conclude that the Jost function $F^+(\lambda_c,k)$ for the superposition of the Coulomb and short-range potentials can be represented as

$$F^+(\lambda_c,k) = B(k^2)f^+(\lambda_c,k) + C(k^2)f^+(\lambda_c,k)\frac{\partial A^+(\lambda,k)}{\partial\lambda}, \tag{10}$$

where $f^+(\lambda_c,k)$ are the Coulomb Jost functions (3), $B(k^2)$ and $C(k^2)$ are analytic functions of k^2, and function $A^+(\lambda,k)$ is defined in Eq. (5). Jost function $F^-(\lambda_c,k)$ can be found from Eq. (10) by means of the well-known symmetry relations [16].

We can use Eq. (10) to solve easily and efficiently the main problem of the QDT: recovering the information about the scattering phase shifts from the known energy levels. We note, first, that since for positive real k the functions $F_{\lambda_c}(k^2,r)$, $\phi_{\lambda_c}(k^2,r)$, and $\phi_{2\lambda_c}(k^2,r)$ are real, the functions $B(k^2)$ and $C(k^2)$ are real there too. Moreover, we know that for the small-k function, $B(k^2)$ is positive. We can consider, therefore, the modified function

$$F_1^+(\lambda_c,k) = f^+(\lambda_c,k) + D(k^2)f^+(\lambda_c,k)\frac{\partial A^+(\lambda,k)}{\partial\lambda}, \tag{11}$$

where $D(k^2) = C(k^2)/B(k^2)$ is a function analytic in some vicinity of $k = 0$. Functions $F_1^+(\lambda_c,k)$ and $F^+(\lambda_c,k)$ clearly have the the same set of zeros in the region near $k = 0$ in the upper half plane, and their phases coincide for real positive k. By the general properties of the Jost functions we mentioned above, $F_1^+(\lambda_c,k)$ has, therefore, zeros in the upper half plane at the points $k_n = i\kappa_n$, where $\kappa_n = 1/\sqrt{-2E_n}$, and E_n are the energies of the bound states. On the real axis for $k > 0$ we have a relation $\delta = -\arg F_1^+(\lambda_c,k)$, where δ is the scattering phase shift.

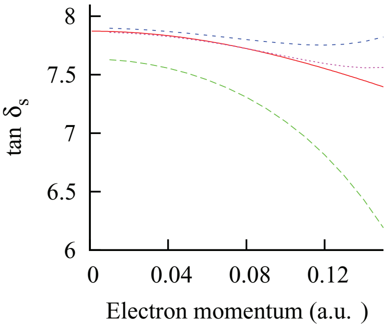

FIG. 1. (Color online) Phase shift δ_s due to the short-range potential for $l = 0$. Results based on the interpolation procedure with nodes corresponding to the levels ns: $n = 4$–7 (green long dashed line), $n = 4$–8 (blue short dashed line), $n = 4$–10 (magenta dots). Red solid line: data obtained by solving the Schrödinger equation with the model potential.

It is extremely easy to devise a scheme which will allow us to extract information about the phase of the $F_1^+(\lambda_c,k)$ provided we know locations of some zeros of this function in the vicinity of $k = 0$. We first compute, according to Eq. (11), values of the analytic function $D(k^2)$ at the points corresponding to the known zeros of $F_1^+(\lambda_c,k)$. There are various ways to approximate an analytic function provided we know its values at a number of points. The most straightforward is, perhaps, a simple Lagrange interpolation, representing $D(k^2)$ as a polynomial in k^2 of some degree equal to the number of points used for interpolation minus one.

This approach is illustrated below using the Li atom. We use the model potential [17] to describe the atom. Using the potential, we find numerically the bound levels and phase shifts. Bound levels' energies and corresponding quantum defects are shown in Table I.

We choose different sets of the bound levels as nodes for the polynomial extrapolation procedure. Results for the phase shift δ_s due to the short-range potential (i.e., total phase shift minus the Coulomb phase shift) are shown in Fig. 1 for s states of Li,

TABLE I. Bound levels' energies and corresponding quantum defects for the ns and np states of Li atom obtained using the model potential [17].

n	E_n (a.u.)	μ_n	E_n (a.u.)	μ_n
	ns		np	
2	−0.1978053	0.4101137	−0.1364203	0.0855435
3	−0.0801823	0.5028439	−0.0600582	0.1146468
4	−0.0402412	0.4750778	−0.0328452	0.0983410
5	−0.0243354	0.4672069	−0.0207862	0.0954690
6	−0.0163168	0.4643701	−0.0143377	0.0946502
7	−0.0117005	0.4629371	−0.0104847	0.0943122
8	−0.0087997	0.4620952	−0.0079997	0.0941446
9	−0.0068582	0.4615533	−0.0063039	0.0940528
10	−0.0054952	0.4611825	−0.0050953	0.0939991
11	−0.0045016	0.4609177	−0.0042037	0.0939653
12	−0.0037550	0.4607225	−0.0035272	0.0939414

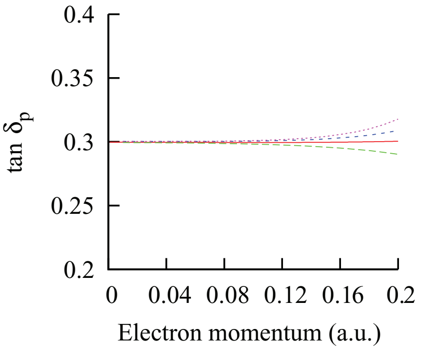

FIG. 2. (Color online) Phase shift δ_s due to the short-range potential for $l = 1$. Results based on the interpolation procedure with nodes corresponding to the levels np: $n = 4$–7 (green long dashed line), $n = 4$–8 (blue short dashed line), $n = 4$–10 (magenta dots). Red solid line: data obtained by solving the Schrödinger equation with the model potential.

and in Fig. 2 for the p states. We see from the figures that the simple Lagrange extrapolation is quite efficient. The accuracy, as the figures show, steadily improves with increasing number of the nodes. This is, of course, what we could have expected since we are solving essentially an extrapolation problem for a function $D(k^2)$ in Eq. (11), which, as we have shown above is a truly analytic analytic function representable by a converging series in k^2. Lagrange extrapolation should represent such functions quite reliably and, as the figures show, this is indeed the case.

III. CONCLUSION

We presented an approach to the QDT theory using the Jost functions and Jost solutions as the main building blocks. An attractive feature of this approach is that we could altogether avoid use of the explicit form of solutions of the radial Schrödinger equation for the Coulomb problem. All we needed to derive Eq. (11) were general analytic properties of the Jost functions and the Jost solutions. Derivation of this result without explicit manipulations with particular Coulomb solutions was, in fact, one of the motivations of this work. Use of the various explicit forms of the Coulomb solutions in the theory leads often to cumbersome expressions, and, more importantly, obscures the physical content of the theory, which, obviously, can not depend on the particular choice of the Coulomb solutions. Note, also, that since we relied mainly on the fairly general properties of the Jost functions and Jost solutions, the procedure can be easily modified to include the case when other long-range interactions (besides Coulomb) are present. In particular, we can consider the case when the long-range part of the potential includes Coulomb and dipole potential A/r^2, for which the Jost functions are known explicitly [18].

Equation (10) gives us a concise representation of the Jost function for the superposition of the Coulomb and short-range potentials. This representation distinctly separates analytic in k terms, and terms singular at $k = 0$. It gives us, therefore, an information about the nature of the singularity of the Jost function (and hence, the intimately related S matrix) at the point $k = 0$, a question which was studied by other means in [12].

The formula for the modified Jost function (11) provides, as we have seen, the basis on which simple and efficient procedures allowing us to determine scattering phase shifts from the information about the bound states can be built. Use of this formula in practice requires a solution of the extrapolation problem for a function $D(k^2)$ in Eq. (11). This function, as we have shown above, is a truly analytic analytic function representable by a converging series in k^2. There is a variety of numerical techniques allowing us to solve this problem accurately and efficiently, starting from the straightforward Lagrange to more accurate Pade extrapolation. As we have seen, even the simplest low-order Lagrange extrapolation procedure gives quite accurate results.

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[1] D. R. Hartree, Math. Proc. Cambridge Philos. Soc. **24**, 89 (1928).
[2] M. Gailitis, Zh. Eksp. Teor. Fiz. **44**, 1974 (1963) [Sov. Phys. JETP **17**, 1328 (1963)].
[3] O. Bely, D. L. Moores, and M. J. Seaton, *Atomic Collision Processes* (North-Holland, Amsterdam, 1963).
[4] M. J. Seaton, Proc. Phys. Soc. **88**, 801 (1966).
[5] M. J. Seaton, J. Phys. B: At. Mol. Phys. **2**, 5 (1969).
[6] M. J. Seaton, J. Phys. B: At. Mol. Phys. **11**, 4067 (1978).
[7] J. Dubau, J. Phys. B: At. Mol. Phys. **11**, 4095 (1978).
[8] U. Fano, Phys. Rev. A **2**, 353 (1970).
[9] C. M. Lee and W. R. Johnson, Phys. Rev. A **22**, 979 (1980).
[10] M. J. Seaton, Rep. Prog. Phys. **46**, 167 (1983).
[11] U. Fano, J. Opt. Soc. Am. **65**, 979 (1975).
[12] V. E. Chernov, N. L. Manakov, and A. F. Starace, Eur. Phys. J. D **8**, 347 (2000).
[13] R. Jost, Helv. Phys. Acta **20**, 256 (1947).
[14] R. Jost and A. Pais, Phys. Rev. **82**, 840 (1951).
[15] P. A. Mari and R. O. Barrachina, J. Phys. B: At. Mol. Phys. **46**, 065202 (2013).
[16] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).
[17] A. Sarsa, F. J. Gálvez, and E. Buendia, At. Data Nucl. Data Tables **88**, 163 (2004).
[18] C. A. López and I. Saavedra, Nucl. Phys. **53**, 519 (1964).