Low-energy expansion of the Jost function for long-range potentials

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(Received 24 March 2006; revised manuscript received 26 May 2006; published 28 November 2006)

The low-energy behavior of the partial-wave Jost function for scattering by a long-range $1/r^s$ ($s>2$) central potential is investigated analytically using the linear variant of the variable-phase equation. An exact expansion of the Jost function in powers of the wave number k is derived iteratively and shown to be simpler compared to the modified effective-range expansion of the phase shift. Improved expansions are determined explicitly for $s=3$ and $s=4$. It is suggested that the Jost function offers a practical alternative for interpolating low-energy cross sections and extracting scattering lengths; this is illustrated by fitting the Jost function, up to a normalizing constant, to the integral cross section for elastic collisions of slow electrons with N_2 molecules.

DOI: 10.1103/PhysRevA.74.052715 PACS number(s): 34.50.−s, 34.80.Bm, 02.30.Zz, 03.65.Nk

I. INTRODUCTION

The low-energy behavior of scattering cross sections can often be summarized by using a small number of parameters such as the scattering length and the effective-range value [1]: the latter was introduced by Bethe [2] in the early days of quantum mechanics in order to interpret low-energy nucleon-nucleon scattering cross sections. Bethe's effective-range expansion for the cotangent of the partial-wave phase shift is only an example of the many low-energy laws which have been developed during the last 50 years for many different types of long-range interactions, and the subject has a long and rich history [3]. Even in the simple case of scattering by a spherically symmetric potential the threshold behavior of the partial-wave phase shifts is trivial only if the potential vanishes at large distances. Much more care is required if the potential exhibits a long-range tail, as is always the case in collisions between charged or polarizable particles such as electrons, atoms, and molecules which at large separations interact via long-range dispersion forces.

In recent years there has been a renewed interest in such expansions due to the impressive progress made in the experimental techniques for cooling and trapping atoms and molecules [4,5]. Using samples of cold atoms or molecules, or mixtures of the two, the long-range interactions between the particles can be studied with an unprecedented accuracy. Progress, albeit less spectacular, has also been made in experiments involving the scattering of slow electrons or positrons by various targets; in particular, it has become possible to produce beams of slow electrons with energies of only a few meV [6].

For a given potential it is in general possible to predict the low-energy behavior of scattering observables; inversely, it is also possible to gather information about the long-range part of the interaction potential by fitting the low-energy expansions to collision data or to extract scattering lengths by extrapolating numerical or experimental data down to threshold [6,7].

If the interaction potential is spherically symmetric and vanishes faster than any power of the distance r, the partial-wave phase shifts can be expanded in odd powers of the collision wave number k. However, if it decreases as $1/r^s$ ($s>2$), the phase shift also contains other powers of k and, in certain cases, logarithmic contributions. These nonanalytic terms have characteristic coefficients that depend on the form of the long-range interaction.

The case of $s=4$ arises when a neutral polarizable system interacts with a charged particle, and it has been extensively studied [8–12]. It seems that the "anomalous" behavior of the partial-wave phase shifts at low energy caused by a $1/r^4$ interaction was first discussed by Thaler [8] in connection with the polarizability of the neutron. Shortly thereafter, O'Malley, Spruch, and Rosenberg [9] showed how Bethe's effective-range theory needs to be modified in this case, and their results have been rederived using different mathematical methods [10,13,14]. The multichannel quantum-defect theory developed by Watanabe and Greene [11] further extends the approach of O'Malley *et al.* to coupled channels and a broader energy range.

The leading term of the Jost function for the case of $2<s\leqslant 3$ has been derived rigorously by Klaus [15], while a repulsive $1/r^3$ interaction has been analyzed in detail by Gao [16]. Several iterative derivations, based on the variable-phase approach and valid for different types of long-range potentials, have also been developed and applied to isotropic [10,17] as well as anisotropic interactions [18,19].

While the semiclassical or JWKB approximation is a powerful method in the case of the Coulomb potential [20], it is less suitable for the dispersion-type potentials that vanish more rapidly than $1/r^2$ [21]. However, still avoiding the use of complicated analytical solutions of the Schrödinger equation, threshold laws and effective-range expansions can be determined in a straightforward manner by treating the long-range part of the potential as a perturbation (see, for example, Sec. 132 of Ref. [21]). The idea is to expand the scattering amplitude or the reactance matrix in a perturbation series which is then truncated at a certain perturbative order, typically the first; the truncated perturbation series is in turn reexpanded in powers and logarithms of k. The method has been used by several authors to derive low-energy expansions for scattering by central potentials vanishing as $1/r^3$ [22], $1/r^4$, $1/r^6$, and $1/r^8$ [23–25] and for a linear combination of a $1/r^4$ and a $1/r^6$ potential [13]. Although an expan-

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sion determined in this manner essentially represents the onset of a perturbation series rather than the onset of an exact series in k, it is known [10,13,18] that the approach results in expansions which are qualitatively correct up to a certain order in k.

More recently Cavagnero [26] developed a secular perturbation theory that can be used to construct analytical low-energy solutions for a $1/r^s$ potential algebraically, and the method has been adopted by Rosenberg [14,27–29] for anisotropic interactions. Rosenberg also presented diagrammatic rules which facilitate the evaluation of higher-order terms of the perturbation series.

Despite the wealth of studies on the subject, it seems that few attempts have been made so far to combine and collect the various laws within a simple and exact formula. We are only aware of a study by van Haeringen and Kok [30] who defined a modified effective-range function which is a meromorphic function of k^2 and which generalizes the more usual effective-range function $k^{2l+1}\cot\delta_l$ associated with scattering by short-range potentials. Unfortunately one does not know in detail how to determine this function explicitly for a given potential. From a fundamental point of view it is certainly unsatisfactory that no explicit, exact low-energy expansion for a general $1/r^s$ long-range potential can be found in the literature.

In this paper we shall show how one can manage to derive an exact series in k for the lth partial-wave Jost function associated with scattering by a central potential vanishing as $1/r^s$ $(s>2)$. We shall focus on the Jost function rather than on the phase shift because of the greater mathematical simplicity of the former. Traditionally one expands the tangent or the cotangent of the phase shift in k: on the other hand, it could be advantageous to use instead the Jost function because the latter often varies less rapidly than, say, the tangent of δ_l [31]. Besides that, the Jost function contains more information than the phase shift alone: it also determines the enhancement factor [1], an important quantity in the theory of final-state interactions [32].

In the spirit of the variable-phase approach to potential scattering [33], we shall define the Jost function $\mathcal{F}_l(k,r)$ for every radial distance r. The asymptotic Jost function is then obtained by taking the limit $r\to\infty$. This formalism, apart from having computational advantages [34,35], allows one to visualize the Jost function's evolution from the origin to $r=\infty$ and therefore lends itself particularly well to theoretical explorations. Since we are interested in the low-energy limit, it is natural to expand the r-dependent Jost function in powers of k and to investigate the long-range behavior of the r-dependent low-energy expansion: thus we are led to define two sets of unknown long-range constants $\alpha_l^{(m)}$ and $\beta_l^{(m)}$ $(m=0,1,2,\ldots)$, which generalize the scattering length and the effective-range parameter: we shall show below that they indeed allow one to express the asymptotic Jost function around $k=0$ in a simple and ordered manner. In order to demonstrate the usefulness of the present approach in practical cases, the resulting general series (29) will then be applied to rederive and extend known expansions for potentials which vanish as $1/r^3$ and $1/r^4$. As a simple application, we shall use the Jost function for the case of $s=4$ in order to interpolate an integral cross section measured recently for electron-N_2 collisions and to deduce from it the scattering length.

Although the present theory has been motivated by recent attempts of using single-channel modified effective-range theory (MERT) in the analysis of beam experiments involving the scattering of slow electrons on biomolecules [6,7,36], our principal aim is here to develop a framework that becomes more useful than those already existing for an in-depth understanding of low-energy scattering by dispersion potentials in general.

In Sec. II the Jost function is therefore cast in the form of a perturbation series; in Sec. III, the low-energy expansion of the asymptotic Jost function is derived, while Sec. IV determines explicitly the initial terms of the expansion for the case of $s=3$ and of $s=4$. In Sec. V the expansions of the phase shift and of the Jost function for $s=4$ are compared by fitting them to an experimental cross section for N_2+e^- collisions. Section VI finally presents our conclusion.

II. PERTURBATION SERIES FOR THE JOST FUNCTION

The radial wave function $u_l(k,r)$ for the lth partial-wave satisfies the Schrödinger equation,

$$\left(\frac{\partial^2}{\partial r^2}+k^2-\frac{l(l+1)}{r^2}-V(r)\right)u_l(k,r)=0, \tag{1}$$

where r is the radial distance and $V(r)$ is the mass-scaled potential. The latter is assumed to be given by

$$V(r)=C_s/r^s \quad (s>2) \tag{2}$$

at large distances. The wave function $u_l(k,r)$ can be normalized such that it is an analytic and even function of k at every distance r. Whenever the potential is less singular at the origin than $1/r^2$, this is ensured by the boundary condition

$$u_l(k,r)\to\frac{j_l(kr)}{k^{l+1}}\to\frac{r^{l+1}}{(2l+1)!!} \quad (r\to 0), \tag{3}$$

where j_l is the Riccati-Bessel function [56]. If the potential is more singular at the origin than $1/r^2$, the origin is an irregular singular point [37] of the Schrödinger equation (1) and the boundary condition (3) is not valid. If the potential is singular and repulsive, the wave function $u_l(k,r)$ can nevertheless be defined such that it is analytic and even in k. Attractive singular potentials, in contrast, pose serious difficulties [38], and we shall exclude them from the present discussion.

At each distance r, we may express the wave function $u_l(k,r)$ as a linear combination of the spherical Riccati-Hankel functions $h_l^{(1)}(x)$ and $h_l^{(2)}(x)$ using two "osculating constants" [37] $F_l^{(1)}(k,r)$ and $F_l^{(2)}(k,r)$ such that

$$u_l(k,r)=\frac{1}{2k^{l+1}}[h_l^{(1)}(kr)F_l^{(1)}(k,r)+h_l^{(2)}(kr)F_l^{(2)}(k,r)], \tag{4}$$

$$\frac{\partial u_l(k,r)}{\partial r} = \frac{1}{2k^l}[h_l^{(1)\prime}(kr)F_l^{(1)}(k,r) + h_l^{(2)\prime}(kr)F_l^{(2)}(k,r)], \quad (5)$$

where a prime indicates the first derivative. This way of matching the wave function and its first derivative to a pair of reference solutions is familiar from the variable-phase method [33]: it guarantees that the coefficients $F_l^{(1)}(k,r)$ and $F_l^{(2)}(k,r)$ become constant at distances where the potential vanishes. Since $u_l(k,r)$ is an even function of k, the coefficients $F_l^{(1)}$ and $F_l^{(2)}$ are not independent: from the parity behavior of the Riccati-Hankel functions it follows that

$$F_l^{(1)}(-k,r) = F_l^{(2)}(k,r) \equiv \mathcal{F}_l(k,r). \quad (6)$$

The coefficient $\mathcal{F}_l(k,r)$, viewed as a function of the wave number k, defines the Jost function for the potential set artificially to zero at distances larger than r, while the Jost function for the true potential is defined as the asymptotic value [1,38,39]

$$\mathcal{F}_l(k,\infty) = \lim_{r\to\infty} \mathcal{F}_l(k,r). \quad (7)$$

In this paper we shall always assume that the wave number k is real. Since it is convenient in this case to use only real-valued quantities, we rewrite Eqs. (4) and (5) using regular and irregular Riccati-Bessel functions j_l and n_l and two osculating constants $A_l(k,r)$ and $B_l(k,r)$,

$$u_l(k,r) = \frac{j_l(kr)}{k^{l+1}}A_l(k,r) - k^l n_l(kr)B_l(k,r), \quad (8)$$

$$\frac{\partial u_l}{\partial r}(k,r) = \frac{j_l'(kr)}{k^l}A_l(k,r) - k^{l+1}n_l'(kr)B_l(k,r). \quad (9)$$

The Jost function is thus rewritten as

$$\mathcal{F}_l(k,r) = A_l(k,r) - ik^{2l+1}B_l(k,r), \quad (10)$$

$$\mathcal{F}_l(-k,r) = A_l(k,r) + ik^{2l+1}B_l(k,r). \quad (11)$$

The variable phase $\delta_l(k,r)$ [33] is determined (up to modulo π) by the ratio $\tan\delta_l(k,r) = k^{2l+1}B_l(k,r)/A_l(k,r)$; it is the phase shift for the potential cut at r. The asymptotic phase shift is $\delta_l(k,\infty)$: as is well known it determines the partial-wave scattering amplitude. The integral cross section of the lth partial wave is then obtained as [1]

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l = 4\pi(2l+1)\frac{k^{4l}B_l^2}{A_l^2 + k^{4l+2}B_l^2}. \quad (12)$$

The coefficients A_l and B_l satisfy a linear version of the variable-phase equation [34,35,40] and are given below in their integral form:

$$A_l(k,r) = A_l(k,d) - \int_d^r dr' k^l n_l(kr')V(r')u_l(k,r'), \quad (13)$$

$$B_l(k,r) = B_l(k,d) - \int_d^r dr' \frac{j_l(kr')}{k^{l+1}}V(r')u_l(k,r'), \quad (14)$$

where d is an arbitrarily fixed distance. The set of Eqs. (8), (13), and (14), is equivalent to the Schrödinger equation (1). The boundary condition (3) is equivalent to $A_l(k,0)=1$ and $B_l(k,0)=0$: these conditions, however, will not be needed in the following discussion.

Iteration of Eqs. (13) and (14), starting with $A^{(0)}(k,r) \equiv A_l(k,d)$ and $B^{(0)}(k,r) \equiv B_l(k,d)$, generates the Neumann series

$$A_l(k,r) = \sum_{n=0}^{\infty} A_l^{(n)}(k,r), \quad (15)$$

$$B_l(k,r) = \sum_{n=0}^{\infty} B_l^{(n)}(k,r), \quad (16)$$

whose members obey the recursion relations

$$A_l^{(n+1)}(k,r) = -\int_d^r dr' k^l n_l(kr')V(r')u_l^{(n)}(k,r'), \quad (17)$$

$$B_l^{(n+1)}(k,r) = -\int_d^r dr' \frac{j_l(kr')}{k^{l+1}}V(r')u_l^{(n)}(k,r'), \quad (18)$$

where

$$u_l^{(n)}(k,r) = \frac{j_l(kr)}{k^{l+1}}A_l^{(n)}(k,r) - k^l n_l(kr)B_l^{(n)}(k,r),$$

$$n = 0,1,2,\ldots . \quad (19)$$

In Appendix A it is shown that $\Sigma_{n=0}^{\infty}A_l^{(n)}(k,r)$ and $k^{2l+2}\Sigma_{n=0}^{\infty}B_l^{(n)}(k,r)$ converge uniformly in k and in r to the solutions $A_l(k,r)$ and $k^{2l+2}B_l(k,r)$. One should note that decoupling Eqs. (13) and (14), as was proposed by Pupyshev [40], is not necessary in our present method: since the series (15) and (16) converge uniformly on the entire radial axis, the asymptotic Jost function is given by the series

$$A_l(k,\infty) = \sum_{n=0}^{\infty} A_l^{(n)}(k,\infty), \quad (20)$$

$$B_l(k,\infty) = \sum_{n=0}^{\infty} B_l^{(n)}(k,\infty). \quad (21)$$

Choosing the distance d to lie in the asymptotic region where the potential has assumed its asymptotic form (2), we may rewrite the series (20) and (21) as

$$\begin{bmatrix} A_l(k,\infty) \\ k^{2l+1}B_l(k,\infty) \end{bmatrix} = \sum_{n=0}^{\infty}(C_s k^{s-2})^n \begin{bmatrix} M_n^{AA}(kd,\infty) & M_n^{AB}(kd,\infty) \\ M_n^{BA}(kd,\infty) & M_n^{BB}(kd,\infty) \end{bmatrix} \times \begin{bmatrix} A_l(k,d) \\ k^{2l+1}B_l(k,d) \end{bmatrix}, \quad (22)$$

where M_0 is the 2×2 unit matrix and the matrices M_n are multiple integrals obeying the recursion relation

$$\begin{bmatrix} M_{n+1}^{AA}(x,t) & M_{n+1}^{AB}(x,t) \\ M_{n+1}^{BA}(x,t) & M_{n+1}^{BB}(x,t) \end{bmatrix} = \int_x^t dt' t'^{-s} \begin{bmatrix} -n_l(t')j_l(t') & n_l(t')n_l(t') \\ -j_l(t')j_l(t') & j_l(t')n_l(t') \end{bmatrix} \times \begin{bmatrix} M_n^{AA}(x,t') & M_n^{AB}(x,t') \\ M_n^{BA}(x,t') & M_n^{BB}(x,t') \end{bmatrix} \quad (n=0,1,2,3,\ldots). \quad (23)$$

(The partial-wave index l on the M_n integrals has been omitted.) The perturbation series (22) maps the value of the Jost function at d into its asymptotic value, and it will be the basis of the low-energy expansion of the next section.

III. LOW-ENERGY EXPANSION

The idea behind the formalism of this section is rather simple. We exploit a peculiar feature of the perturbation series (22): its repeated integrals depend on the wave number k only through the product kd. In fact this implies that an expansion of any of these integrals in powers of k is also an expansion in powers of d. The limiting value of the series (22) (i.e., the asymptotic Jost function), on the other hand, does not depend on the choice of d. Therefore, when the integrals in Eq. (22) are expanded around $k=0$, we certainly need to retain only terms of zero order in d, provided that the values $A_l(k,d)$ and $B_l(k,d)$ can also be expanded in powers and logarithms of d.

Since we are interested in the low-energy behavior of the asymptotic values $A_l(k,\infty)$ and $B_l(k,\infty)$, we must investigate limits for both $k\to 0$ and $r\to\infty$. First of all we note that the wave function $u_l(k,r)$ and the basis functions $j_l(kr)/k^{l+1}$ and $k^l n_l(kr)$ in Eqs. (8) and (9) are all analytic and even functions of the wave number k: this means that the coefficients $A_l(k,r)$ and $B_l(k,r)$ are also analytic and even in k. At each finite distance r we can therefore expand them in k^2,

$$A_l(k,r) = \sum_{m=0}^{\infty} a_l^{(m)}(r)k^{2m}, \quad (24)$$

$$B_l(k,r) = \sum_{m=0}^{\infty} b_l^{(m)}(r)k^{2m}. \quad (25)$$

By expanding also the reference functions $j_l(kr)/k^{l+1}$ and $k^l n_l(kr)$ in k^2, one sees that $a_l^{(m)}(r)$ and $b_l^{(m)}(r)$ $(m=0,1,2,\ldots)$ solve a recursive linear system of coupled first-order differential equations. Similar equations for the variable phase have been studied before by Levy and Keller [10] and by Ali and Fraser [17].

In the case of $s<2l+3$ the zero-energy functions $a_l^{(0)}(r)$ and $b_l^{(0)}(r)$ tend to finite limits $a_l^{(0)}(\infty)$ and $b_l^{(0)}(\infty)$ in the asymptotic limit $r\to\infty$. From Eq. (8) it then follows that the zero-energy wave function behaves asymptotically as

$$u_l(0,r) \to \frac{r^{l+1}}{(2l+1)!!}a_l^{(0)}(\infty) + \frac{(2l+1)!!}{2l+1}r^{-l}b_l^{(0)}(\infty) \quad (26)$$

and the partial-wave scattering length is then defined as the ratio $-b_l^{(0)}(\infty)/a_l^{(0)}(\infty)$ [21].

Generally, however, the functions $a_l^{(m)}(r)$ and $b_l^{(m)}(r)$ $(m=0,1,2,\ldots)$ diverge (unless $C_s=0$), so that the asymptotic Jost function cannot be obtained from Eqs. (24) and (25) by simply taking the limit $r\to\infty$. Nevertheless one may expect that the expansions of $A_l(k,\infty)$ and $B_l(k,\infty)$ in k are intimately linked to the long-range behavior of $a_l^{(m)}(r)$ and $b_l^{(m)}(r)$. The long-range asymptotic forms of $a_l^{(m)}(r)$ and $b_l^{(m)}(r)$ $(m=0,1)$ are given in Appendix B for the special case of $s=3$, $l=0$. Similar forms exist for the general case of $s>2$ and arbitrary $l=0,1,2,\ldots$. One sees that $a_l^{(m)}(r)$ and $b_l^{(m)}(r)$ can both be expanded in powers and in logarithms of r—i.e., in the functions $r^p \ln^q(r/\rho)$, $(p,q)\in\mathbb{R}^2$ where ρ is a constant length that we have introduced only in order to obtain a dimensionless quantity r/ρ and which can be chosen freely.

For future convenience, the zero order terms of the long-range forms $a_l^{(m)}(r)$ and $b_l^{(m)}(r)$ will be called $\alpha_l^{(m)}$ and $\beta_l^{(m)}$ $(m=0,1,2,\ldots)$. Note that they are not necessarily the leading terms. Furthermore, they depend on the choice made for ρ if $a_l^{(m)}(r)$ and $b_l^{(m)}(r)$ contain terms of logarithmic order in r [note the identity $\ln(r/\rho)=\ln(r/\rho')+\ln(\rho'/\rho)$]. The explicit example of Eq. (B9) in Appendix B, or a dimensional analysis, then suggest that the long-range forms of $a_l^{(m)}(r)$ and $b_l^{(m)}(r)$ can be compactly written as

$$\begin{bmatrix} A_l(k,r) \\ k^{2l+1}B_l(k,r) \end{bmatrix} = \sum_{n=0}^{\infty} (C_s k^{s-2})^n \begin{bmatrix} Q_n^{AA}(k,r) & Q_n^{AB}(k,r) \\ Q_n^{BA}(k,r) & Q_n^{BB}(k,r) \end{bmatrix} \times \begin{bmatrix} \alpha_l^{(0)} + \alpha_l^{(1)}k^2 + Ok^4 \\ \beta_l^{(0)}k^{2l+1} + \beta_l^{(1)}k^{2l+3} + Ok^{2l+5} \end{bmatrix}, \quad (27)$$

where $Q_0(k,r)$ is the 2×2 identity matrix and the matrices $Q_{n'}(k,r)$ $(n'>1)$ expand in nonzero powers of kr and possibly in logarithms of r/ρ. (The symbol O means "the order of.") The Q_n matrices can be generated by iterating the differential version of the variable-phase equations (13) and (14) after expanding the equations in k (or in $x=kr$), and by absorbing all integration constants in the $\alpha_l^{(m)}$ and $\beta_l^{(m)}$ constants.

Inserting the long-range form (27) in the perturbation series (22) then gives the double series

$$\begin{bmatrix} A_l(k,\infty) \\ k^{2l+1}B_l(k,\infty) \end{bmatrix} = \sum_{n,n'=0}^{\infty} (C_s k^{s-2})^{n+n'} \times \begin{bmatrix} M_n^{AA}(kd,\infty) & M_n^{AB}(kd,\infty) \\ M_n^{BA}(kd,\infty) & M_n^{BB}(kd,\infty) \end{bmatrix} \times \begin{bmatrix} Q_{n'}^{AA}(k,d) & Q_{n'}^{AB}(k,d) \\ Q_{n'}^{BA}(k,d) & Q_{n'}^{BB}(k,d) \end{bmatrix} \times \begin{bmatrix} \alpha_l^{(0)} + \alpha_l^{(1)}k^2 + Ok^4 \\ \beta_l^{(0)}k^{2l+1} + \beta_l^{(1)}k^{2l+3} + Ok^{2l+5} \end{bmatrix}, \quad (28)$$

where $M_n(kd,\infty)$ expands in powers and logarithms of kd while $Q_n(k,d)$ expands in powers of kd and logarithms of d/ρ. The leading terms of the above series are given explicitly in Eqs. (B15) and (C1) of the Appendix for two specific cases, $s=3$ and $s=4$. We may immediately simplify Eq. (28) by noting that the sum on the right-hand side cannot depend on d: in fact all terms of nonzero order in d must cancel exactly when the expansions for $M_n(kd,\infty)$ and $Q_{n'}(k,d)$ are multiplied out. We thus obtain our principal result,

$$\begin{bmatrix} A_l(k,\infty) \\ k^{2l+1}B_l(k,\infty) \end{bmatrix} = \sum_{n=0}^{\infty} (C_s k^{s-2})^n \begin{bmatrix} L_n^{AA}(k\rho) & L_n^{AB}(k\rho) \\ L_n^{BA}(k\rho) & L_n^{BB}(k\rho) \end{bmatrix} \times \begin{bmatrix} \alpha_l(k) \\ k^{2l+1}\beta_l(k) \end{bmatrix}, \tag{29}$$

where the 2×2 matrices $L_n(x)$ $(n=0,1,2,\ldots)$ are obtained by multiplying out the expansions of the perturbation integrals and of the long-range forms in Eq. (28) and where we have defined the functions

$$\alpha_l(k) = \sum_{m=0}^{\infty} \alpha_l^{(m)} k^{2m}, \tag{30}$$

$$\beta_l(k) = \sum_{m=0}^{\infty} \beta_l^{(m)} k^{2m} \tag{31}$$

via their expansions around $k=0$.

It is very important to note that the matrices L_n $(n=0,1,2,\ldots)$ in Eq. (29) are either *constants* or depend only *logarithmically* on k: in fact, in Eq. (28) a term of order $(kd)^p$ stemming from the perturbation integrals must be multiplied with a term of order $(kd)^{-p}$ in the long-range form of the Jost function to yield a term of zero order in d, and the product $(kd)^p(kd)^{-p}$ does obviously not depend on k. L_n may still depend logarithmically on k because a logarithmic term $\ln(kd)$ stemming from the perturbation integrals splits as $\ln(k\rho)+\ln(d/\rho)$—i.e., into a term that only depends on k and a term that only depends on d: in this case the k-dependent part remains present in Eq. (28) while the d-dependent term must cancel with some other term that also depends logarithmically on d.

The matrices L_0, L_1, and L_2 are given more explicitly by

$$L_0(k\rho) = 1, \tag{32}$$

$$L_1(k\rho) = Q_1(k,d) + M_1(kd,\infty), \tag{33}$$

$$L_2(k\rho) = Q_2(k,d) + M_1(kd,\infty)Q_1(k,d) + M_2(kd,\infty). \tag{34}$$

Since the above expressions do not depend on d, a finite number of terms in the expansions of $M_n(kd,\infty)$ and $Q_{n'}(k,d)$ is sufficient to determine $L_n(k\rho)$ for a given order of n. In particular, the first-order correction L_1 given by (33) coincides with the term of constant or logarithmic order in the expansion of the perturbation integral $M_1(x,\infty)$ around $x=0$.

An explicit evaluation of the $L_n(x)$ functions in Eq. (29) for higher orders of n is difficult because it requires analyzing the repeated integrals of the perturbation series (22). In Sec. IV, we shall, however, evaluate the first- and second-order terms, L_1 and L_2, for the case of s-wave scattering by potentials which vanish as $1/r^3$ and as $1/r^4$.

We introduced the series $\alpha_l(k)$ and $\beta_l(k)$ defined in Eqs. (30) and (31) mainly in order to simplify the notation, without proving their convergence, and in principle it might be possible that they both diverge (unless $k=0$). In this case the series (29) remains well-defined provided that its terms are summed in the order of increasing powers of k using the well-defined coefficients $\alpha_l^{(m)}$ and $\beta_l^{(m)}$. Similarly one may wonder whether the 2×2 matrix series $\Sigma_n(C_s k^{s-2})^n L_n(k\rho)$ converges alone: these are mathematical issues that would merit further attention. For the moment it is probably safer to regard Eq. (29) as a series in k rather than as a series in $C_s k^{s-2}$ since it stems from an expansion of the perturbation series (22) in powers of k: note that it is simple enough to be truncated at any desired order in k, the functions $L_n(x)$ being either constants or diverging only logarithmically for $x\to 0$.

In the case of $C_s=0$, the series (29) reduces to the usual Taylor series for the Jost function around $k=0$, while in the presence of a long-range interaction $(C_s\neq 0)$ the Taylor series is modified by nonanalytic functions. It should be noted, however, that the long-range constants encoded in $\alpha_l(k)$ and $\beta_l(k)$ implicitly depend on the C_s coefficient: in fact one may expect that both $\alpha_l(k)$ and $\beta_l(k)$ are quite sensitive to the long-range part of the potential since they generalize the scattering length.

By retaining in Eq. (29) only the leading terms for $k\to 0$ the threshold behavior of the partial-wave Jost function is seen to be

$$\mathcal{F}_l(k,\infty) \sim \begin{cases} \alpha_l^{(0)} - ik^{2l+1}\beta_l^{(0)} & \text{if } 2l+3 < s, \\ \alpha_l^{(0)} - ik^{2l+1}[\beta_l^{(0)} + C_s L_1^{BA}(k\rho)\alpha_l^{(0)}] & \text{if } 2l+3 = s, \\ \alpha_l^{(0)} - iC_s k^{s-2} L_1^{BA}(k\rho)\alpha_l^{(0)} & \text{if } s < 2l+3. \end{cases} \tag{35}$$

The above equation holds for the general case of $\mathcal{F}_l(0,\infty)\neq 0$. In the special case of $\mathcal{F}_l(0,\infty)=0$, the series (29) remains valid, but its leading terms then differ from those in Eq. (35).

On the other hand, the present derivation does not allow us to give a general estimate for the maximum energy value up to which the series (29), truncated after a certain order in k, will be a useful approximation. The reason for this is that the constants $\alpha_l^{(m)}$ and $\beta_l^{(m)}$ $(m=0,1,2,\ldots)$ in Eqs. (30) and (31) are defined "at infinity;" i.e., they summarize the accumulated effects of the potential from the origin to $r\to\infty$ and may therefore be fairly large, an hypothesis that is confirmed numerically in Sec. V for a concrete case. Finding some estimate would certainly require more knowledge about the details of the specific physical system: it would at least be necessary to know the distance at which the potential takes up its long-range form. It is a recognized problem in potential scattering that effective-range expansions are usually valid only within a very small energy range near threshold

[3,12,16], although the expansions can be extended to higher energies by including higher powers of k, a procedure which also requires using more parameters (long-range constants $\alpha_l^{(m)}$ and $\beta_l^{(m)}$ in our method). It therefore follows that in order to predict or to explain the behavior of scattering observables over larger energy domains other methods like quantum-defect theory [41,42] may be better suited (see also our remarks in the concluding Sec. VI).

In many situations (e.g., elastic scattering) the physically relevant information is contained in the phase shift alone and the complete Jost function is then not needed. The expansion of $\tan \delta_l(k,\infty)$ around $k=0$ is found from Eq. (29) by equating like powers of $C_s k^{s-2}$ on both sides of the identity

$$\tan \delta_l(k,\infty) A_l(k,\infty) = k^{2l+1} B_l(k,\infty).$$

To order $(C_s k^{s-2})^2$ we thus obtain

$$\begin{aligned}\tan \delta_l(k,\infty) = &- k^{2l+1}\lambda_l(k) + L_1^{BA} C_s k^{s-2} + (L_1^{AA} \\ &- L_1^{BB}) C_s k^{s+2l-1}\lambda_l(k) - L_1^{AB} C_s k^{s+4l}\lambda_l(k)^2 + (L_2^{BA} \\ &- L_1^{BA} L_1^{AA}) C_s{}^2 k^{2s-4} + (L_2^{AA} - L_2^{BB} + L_1^{AB} L_1^{BA} \\ &+ L_1^{AA} L_1^{BB} - L_1^{AA} L_1^{AA}) \times C_s{}^2 k^{2s+2l-3}\lambda_l(k) \\ &+ (2L_1^{AA} L_1^{AB} - L_1^{AB} L_1^{BB} - L_2^{AB}) C_s{}^2 k^{2s+4l-2}\lambda_l(k)^2 \\ &- L_1^{AB} L_1^{AB} C_s{}^2 k^{2s+6l-1}\lambda_l(k)^3 + O C_s{}^3 k^{3s-6-\epsilon}, \quad (36)\end{aligned}$$

where we have suppressed the argument $k\rho$ of the logarithmic terms $L_n(k\rho)$ and where we have introduced the ratio

$$\lambda_l(k) = -\frac{\beta_l(k)}{\alpha_l(k)} \quad (37)$$

which expands in even powers of k,

$$\lambda_l(k) = \lambda_l^{(0)} + \lambda_l^{(1)} k^2 + \lambda_l^{(2)} k^4 + \cdots . \quad (38)$$

In the case of $2l+3<s$, the coefficient $\lambda_l^{(0)} = \lambda_l(0)$ is the scattering length as defined by the long-range asymptotic form of the zero-energy wave function (26), while $\lambda_l^{(1)}$ is a quantity analogous to the effective-range parameter. In the special case of $\alpha_l(0)=0$ the scattering length becomes infinite.

The first two terms in Eq. (36), i.e.,

$$\tan \delta_l(k,\infty) \sim - k^{2l+1}\lambda_l(k) + L_1^{BA}(k\rho) C_s k^{s-2} \quad (39)$$

essentially summarize Eqs. (67), (68), and (69) of Levy's and Keller's historical paper [10]. In the particular case of $2l+3>s$, the function $L_1^{BA}(x)$ [i.e., the term of order $x^{-\epsilon}$ in the expansion of $M_1^{BA}(x,\infty)$ around $x=0$] can be determined explicitly by splitting $M_1^{BA}(x,\infty)$ as

$$M_1^{BA}(x,\infty) = -\int_0^\infty t^{-s}[j_l(t)]^2 dt + \int_0^x t^{-s}[j_l(t)]^2 dt. \quad (40)$$

The two integrals on the right-hand side are of orders 1 and x^{2l+3-s}, respectively, so that $L_1^{BA}(x)$ is seen to coincide with the first one, which is known analytically [10]:

$$L_1^{BA}(x) = -\int_0^\infty t^{-s}[j_l(t)]^2 dt \quad (41)$$

$$= -\frac{\pi}{2}\int_0^\infty t^{1-s}[J_{l+1/2}(t)]^2 dt \quad (42)$$

$$= -\frac{\pi}{2^s}\frac{\Gamma(s-1)\Gamma\left(l+\frac{3}{2}-\frac{1}{2}s\right)}{\Gamma^2\left(\frac{1}{2}s\right)\Gamma\left(l+\frac{1}{2}+\frac{1}{2}s\right)},$$

$$2 < s < 2l+3. \quad (43)$$

Similarly, the term $(L_2^{BA} - L_1^{BA} L_1^{AA}) C_s{}^2 k^{2s-4}$ in Eq. (36) is the second-order contribution that has been evaluated by Wadehra [43] for the case of $2l+5>2s$.

Since no approximation has been made in the present derivation, we believe that the series for the Jost function (29) is exact within its (unknown) radius of convergence. We should point out that a simpler perturbative treatment, starting from a truncated perturbation series, would have led to a scattering length that is correct only to a certain perturbative order [13]: in fact the term of order k^{2l+1} in Eq. (36) can also be obtained in an approximate manner by truncating the perturbation series (22) after a finite number of iterations and by then expanding the truncated series in k. For example, truncating Eq. (22) after zero iterations—i.e., neglecting completely the long-range part of the potential—would give $k^{2l+1} B_l(0,d)/A_l(0,d)$ instead of the exact value $k^{2l+1}\beta_l^{(0)}/\alpha_l^{(0)}$. If the ratio $B_l(0,d)/A_l(0,d)$ is only used as a fitting parameter, there is nothing wrong with using this approximation, since replacing it by the correct numerical value of the scattering length gives the correct threshold law. Similarly we know that the modified effective-range expansions obtained in first order in the interaction strength [13,22,24,25] are useful fitting formulas up to a certain order in k. Therefore, it is important to note that the $\alpha_l^{(m)}$ and $\beta_l^{(m)}$ coefficients ($m=0,1,2,\ldots$) in the series (29) are not defined implicitly by the series itself but, in a rather simple manner, by the asymptotic long-range behavior of the wave function.

One notices that the "modified effective-range expansion" (29) for the Jost function is *very much simpler* than the corresponding formula (36) for the phase shift: while (α_l, β_l) is mapped linearly to (A_l, B_l), $\tan \delta_l$ depends on $\lambda_l(k)$ in a nonlinear manner due to the presence of higher powers of $\lambda_l(k)$. This result is not surprising, considering that the variable-phase equations for A_l and B_l are linear whereas the equation for $\tan \delta_l(k,r)$ is nonlinear. The occurrence of higher powers of $\lambda_l(k)$ in the threshold law (36) for $\tan \delta_l$ is certainly not an artifact of our derivation: in fact the higher-order expansions for $s=4$ derived recently by Rosenberg [14] and by Macri and Barrachina [12] also contain higher powers of the scattering length and terms mixing the scattering length and the effective-range parameter. Although it has become customary to expand $\tan \delta_l$ or $\cot \delta_l$ explicitly in powers and logarithms of k, it seems therefore more natural to express $\tan \delta_l$ as the ratio $k^{2l+1} B_l(k,\infty)/A_l(k,\infty)$, the expansions of A_l and B_l being so much simpler.

Another argument for using the Jost function is the following. Let us assume that $A_l(k,\infty)$ and $B_l(k,\infty)$ are well

approximated within a certain energy range by the series (29) truncated after some finite order of $C_s k^{s-2}$. Then the tangent is of course well approximated by the ratio $k^{2l+1}B_l/A_l$ using the truncated series for A_l and B_l. In contrast higher powers of $C_s k^{s-2}$ would in general be needed in the explicit expansion (36) of $\tan\delta_l$ in order to achieve the same level of accuracy [57]. This will be particularly the case in the vicinity of energies at which the phase shift passes through 90°. Using the Jost function in the form of Eq. (29) it could therefore be possible to extend the energy domain in which modified effective-range theory is applicable.

IV. SPECIFIC EXPANSIONS: $s=3$ AND $s=4$

We have evaluated our series (29) for two cases of physical interest—i.e., for $s=4$ and $s=3$—in both cases truncating it after $n=2$. We shall also indicate the corresponding expansions of $\tan\delta_l$, although, as we mentioned in the preceding section, it may often be more convenient to express $\tan\delta_l$ in terms of the Jost function.

The algebraic details are given in Appendixes B and C.

A. The case of $s=3$, $l=0$

A spherically symmetric $1/r^3$ interaction can occur between two identical particles such as an S and a P state atom of the same species [21]. Anisotropic $1/r^3$ potentials are encountered more frequently in nature as they include dipole-dipole and charge-quadrupole interactions [19]; we should therefore point out that the results established here are valid only for an isotropic interaction, although the formalism can be generalized to anisotropic forces.

For the case of $s=3$, $l=0$, the series (29) becomes

$$A_0(k,\infty)=\left\{1-\frac{\pi}{2}C_3k+\frac{1}{2}\left[\left(\ln 2k\rho+\gamma-\frac{5}{3}\right)^2-1+\frac{\pi^2}{4}\right]C_3^2k^2+OC_3^3k^{3-\epsilon}\right\}\alpha_0(k)+\left[\left(\ln 2k\rho+\gamma-\frac{3}{2}\right)C_3k-\frac{\pi}{2}\left(\ln 2k\rho+\gamma-\frac{4}{3}\right)C_3^2k^2+OC_3^3k^{3-\epsilon}\right]k\beta_0(k), \tag{44}$$

$$kB_0(k,\infty)=\left[\left(\ln 2k\rho+\gamma-\frac{3}{2}\right)C_3k+\frac{\pi}{2}\left(\ln 2k\rho+\gamma-\frac{5}{3}\right)C_3^2k^2+OC_3^3k^{3-\epsilon}\right]\alpha_0(k)+\left\{1+\frac{\pi}{2}C_3k+\frac{1}{2}\left[\left(\ln 2k\rho+\gamma-\frac{4}{3}\right)^2-\frac{14}{9}+\frac{\pi^2}{4}\right]C_3^2k^2+OC_3^3k^{3-\epsilon}\right\}k\beta_0(k), \tag{45}$$

where $\gamma=0.577\,22\cdots$ is the Euler-Mascheroni constant and $\alpha_0(k)$ and $\beta_0(k)$ expand in even powers of k, as explained in Sec. III. Using Eqs. (B10)–(B14) of Appendix B, we have checked to order $k^2C_3^2$ that the form of Eqs. (44) and (45) remains unchanged in a transformation $\rho\to\rho'$.

In the ordinary case of $A_0(0,\infty)\neq 0$, Eqs. (44) and (45) extend the leading term derived by Klaus [15] to higher order in k. In the special case of $A_0(0,\infty)=0$, however, the leading term of $A_0(k,\infty)$ is twice as large as predicted by Klaus who treated this case separately. A possible explanation for this discrepancy is given in Appendix B.

Using Eq. (36) we furthermore obtain the following expansion in k for the tangent of the s-wave phase shift:

$$\tan\delta_0(k,\infty)=\left[-\lambda_0(k)+\left(\ln 2k\rho+\gamma-\frac{3}{2}\right)C_3\right]k+\pi\left[-\lambda_0(k)+\left(\ln 2k\rho+\gamma-\frac{19}{12}\right)C_3\right]C_3k^2-\left(\ln 2k\rho+\gamma-\frac{3}{2}\right)C_3\lambda_0(k)^2k^3+\left[\left(\ln 2k\rho+\gamma-\frac{5}{3}\right)^2+\frac{1}{4}-\frac{\pi^2}{2}\right]C_3^2k^3-\pi\left(\ln 2k\rho+\gamma-\frac{19}{12}\right)C_3^2\lambda_0(k)^2k^4-\left(\ln 2k\rho+\gamma-\frac{3}{2}\right)^2C_3^2\lambda_0(k)^3k^5+OC_3^3k^{3-\epsilon} \tag{46}$$

which extends to second order in k the threshold law derived by Shakeshaft [22]: it contains several terms of second order in the interaction strength; note in particular the contribution $C_3^2k^2\pi\left(\ln 2k\rho+\gamma-\frac{19}{12}\right)$ which dominates over the usual k^3 term at low energies. This new term is interesting because it improves the threshold law in the ultralow-energy range in which the phase shift is essentially determined by the "generalized scattering length" $\lambda_0(0)$. It should be noted that Shakeshaft's expansion of $\tan\delta_0$, given by Eq. (5) of Ref. [22], depends on two correlated parameters d and A_0 in such a way that changing d alters the coefficient of the k^2 term if the leading term, $k\times(\text{const}+C_3\ln kd)$, is to remain unchanged. This clearly shows that Eq. (5) in Ref. [22] is correct only to first order in k. Here we have instead derived a formula which is exact up to and including order k^2, and it is obvious that Eq. (46), truncated after order k^2, does not change its form if we rescale $\rho\to\rho'$, provided that we also make the substitution $\lambda_0(k)\to\lambda_0'(k)\equiv\lambda_0(k)+\ln(\rho'/\rho)C_3$. This invariance further confirms the exactitude of many of the algebraic constants in Eqs. (44) and (45) which we calculated "by hand" and which are quite difficult to verify otherwise. The contributions of order $C_3k^{3-\epsilon}$ and higher have been retained in Eq. (46) only for the sake of completeness: in reality they compete with terms of third perturbative order which we did not attempt to evaluate.

The threshold behavior of $\tan\delta_l$ has also been discussed by Gao [16] for the particular case of a purely repulsive $1/r^3$ potential. Since Eq. (59) in Ref. [16] is exact only to first order in kC_3, we may rewrite it as

$$\tan\delta_0=kC_3\left[\ln(2kC_3)+3\gamma-\tfrac{3}{2}\right]+O(kC_3)^{2-\epsilon}, \tag{47}$$

which is a special case of our more general expression (46): it corresponds to the value $\lambda_0(0)=-[\ln(C_3/\rho)+2\gamma]C_3$. While Gao's expression is parameter free, our Eq. (46) is valid for both repulsive and attractive interactions and also for the more realistic situation in which the potential deviates at short distances from its long-range $1/r^3$ form: the price to

pay for this increased generality is the need for the function $\lambda_0(k)$ of which we only know that it expands in k^2.

From Eq. (46) one may further obtain the s-wave integral cross section: as is well known [3,21] it diverges logarithmically for $k \to 0$.

B. The case of $s=4$

The prominent example of an isotropic $1/r^4$ potential is the charge-induced dipole interaction between a charged particle and a neutral, polarizable system—for example, an electron and an atom or a molecule. Although the effects of such a potential on low-energy scattering phase shifts have been extensively studied [9,10,14,26,28,44], the threshold behavior of the Jost function has been derived only fairly recently by Macri and Barrachina [12] by using the detailed properties of the Mathieu functions. Here we rederive it (and extend it to slightly higher order in k) using the perturbative approach.

For the case of $s=4$, $l=0$, the series (29) takes the form

$$A_0(k,\infty) = \left\{1 + \frac{2}{3}\left(\ln 2k\rho + \gamma - \frac{11}{6}\right)C_4k^2 + \frac{2}{9}\left[\left(\ln 2k\rho + \gamma - \frac{9}{5}\right)^2 - \frac{983}{900} + \frac{\pi^2}{4}\right]C_4^2k^4 + OC_4^3k^{6-\epsilon}\right\}\alpha_0(k) + \left[\frac{\pi}{3}C_4k^2 - \frac{2\pi}{9}\left(\ln 2k\rho + \gamma - \frac{28}{15}\right)C_4^2k^4 + OC_4^3k^{6-\epsilon}\right]k\beta_0(k), \tag{48}$$

$$kB_0(k,\infty) = \left[\frac{\pi}{3}C_4k^2 + \frac{2\pi}{9}\left(\ln 2k\rho + \gamma - \frac{9}{5}\right)C_4^2k^4 + OC_4^3k^{6-\epsilon}\right]\alpha_0(k) + \left\{1 - \frac{2}{3}\left(\ln 2k\rho + \gamma - \frac{11}{6}\right)C_4k^2 + \frac{2}{9}\left[\left(\ln 2k\rho + \gamma - \frac{28}{15}\right)^2 - \frac{889}{900} + \frac{\pi^2}{4}\right]C_4^2k^4 + OC_4^3k^{6-\epsilon}\right\}k\beta_0(k), \tag{49}$$

while the expansion (36) for the tangent of the s-wave phase shift is now given by

$$\tan\delta_0(k,\infty) = -k\lambda_0(k) + \frac{\pi}{3}C_4k^2 + \frac{4}{3}\left(\ln 2k\rho + \gamma - \frac{11}{6}\right)C_4k^3\lambda_0(k) - \frac{\pi}{3}C_4k^4\lambda_0(k)^2 + \frac{\pi}{135}C_4^2k^4 - \frac{8}{9}\left[\left(\ln 2k\rho + \gamma - \frac{37}{20}\right)^2 + \frac{31}{1200} - \frac{\pi^2}{8}\right]C_4^2k^5\lambda_0(k) + \frac{8\pi}{9}\left(\ln 2k\rho + \gamma - \frac{221}{120}\right)C_4^2k^6\lambda_0(k)^2 - \frac{\pi^2}{9}C_4^2k^7\lambda_0(k)^3 + OC_4^3k^{6-\epsilon}; \tag{50}$$

it extends the O'Malley-Spruch-Rosenberg modified effective-range expansion [9] to higher powers in k. The unknown function $\lambda_0(k)$ expands in powers of k^2 and can be adjusted to experimental data for a given physical system. It should be mentioned that Eq. (50) gives the Fk^4 term of Buckman's and Mitroy's MERT5 expansion [45] exactly: in fact F is determined entirely by the scattering length and the polarizability.

Equations (48) and (50) confirm Macri and Barrachina's expansions [12], and they could also be recovered from Watanabe and Greene's theory [11] which also makes use of Jost functions. Some of the higher-order terms in Eq. (50) have also been known before, at least approximately, from Rosenberg's variational study [14]. Our equations are simpler in appearance, both compared to Macri and Barrachina [12] and to Rosenberg [14], because we have encoded all unknown parameters in the Taylor series for $\alpha_0(k)$ and $\beta_0(k)$: once more we emphasize that these parameters are not arbitrary but have been defined in Sec. III via the long-range behavior of the wave function.

The first-order corrections to the threshold law of the Jost function for higher partial waves ($l \geqslant 1$) can also be found analytically (see again Appendix C). In particular, for the p wave we write

$$A_1(k,\infty) = \left[1 - \frac{2}{15}\left(\ln 2k\rho + \gamma - \frac{31}{30}\right)C_4k^2 + OC_4^2k^{4-\epsilon}\right]\alpha_1(k) + \left(-\frac{\pi}{15}C_4k^2 + OC_4^2k^{4-\epsilon}\right)k^3\beta_1(k), \tag{51}$$

$$k^3B_1(k,\infty) = \left(-\frac{\pi}{15}C_4k^2 + OC_4^2k^{4-\epsilon}\right)\alpha_1(k) + \left[1 + \frac{2}{15}\left(\ln 2k\rho + \gamma - \frac{31}{30}\right)C_4k^2 + OC_4^2k^{4-\epsilon}\right]k^3\beta_1(k) \tag{52}$$

and accordingly, for the phase shift,

$$\tan\delta_1(k,\infty) = -k^3\lambda_1(k) - \frac{\pi}{15}C_4k^2 - \frac{4}{15}\left(\ln 2k\rho + \gamma - \frac{31}{30}\right)C_4k^5\lambda_1(k) + \frac{\pi}{15}C_4k^8\lambda_1(k)^2 + OC_4^2k^4. \tag{53}$$

The terms linear in C_4 that appear in Eqs. (50) and (53) are all well known from Hinckelmann and Spruch's first-order perturbative analysis [13]. The derivation in Ref. [13] was, however, unnecessarily complicated as the "d-dependent terms" we discussed in Sec. III were regrouped only in the very final step, whereas we rearranged them at an early stage so that they are no longer explicitly present in our series (29).

V. APPLICATION TO ELASTIC N_2-ELECTRON COLLISIONS

Field has kindly provided us with an experimental integral cross section for scattering of slow electrons on N_2 molecules in the energy range from 10 meV to 0.7 eV [46]. In order to test some of the explicit expansions derived above, we have fitted both the partial-wave Jost functions and the partial-wave phase shifts for $l=0$ and $l=1$ to this cross section. A more stringent test would require precise numerical data for the phase shifts or the reactance matrix.

The threshold for excitation from the vibrational ground state to the N_2 $(v=1,\ j=0)$ vibrational level lies at 2327.13 cm^{-1}—that is, 0.288 527 eV. The collision between e^- and N_2 is therefore a multichannel problem, involving both rotational and vibrational degrees of freedom. However, the inelastic cross section is known to be very small [47–49] in the low-energy range ($E \leqslant 0.7$ eV) considered here. We therefore make the simplifying assumption that the electron essentially "sees" a spherically symmetric target with no internal structure, a simplification which has been successfully used before to interpret several electron-molecule collision experiments [6,7,36,47].

The spherical polarizability of N_2 is known to be $-C_4 = 11.8$ a.u. [48], and the reduced atom-molecule interaction potential behaves asymptotically as $V(r)=C_4/r^4$. The value of the polarizability can also be deduced quite accurately from the experimental cross section by fitting it together with the scattering length using only the leading terms of the modified effective-range expansion [9]. However, in the following C_4 will be taken constant.

The energy range of 10 meV $< E <$ 0.7 eV covered by the experiment is such that only the s- and p-wave phase shifts are expected to be important: in fact, Eqs. (39) and (43) with $s=4$ indicate that at an energy of 0.7 eV the d-wave partial cross section is negligible. We therefore approximate the integral cross section σ as the sum of the s- and p-wave partial cross sections, $\sigma=\sigma_1+\sigma_2$. In order to extract phase shifts from the experimental cross section, we express the partial cross sections σ_l $(l=0,1)$ in terms of either $\tan\delta_l$ or the Jost function. The latter is expressed in terms of the real functions A_l and B_l $(l=0,1)$. We then substitute for $\tan\delta_0$ and $\tan\delta_1$ the low-energy forms (50) and (53), and similarly we use for the Jost function the forms (48), (49), (51), and (52). In order to simplify our formulas we choose the unit length ρ such that $\ln 2k\rho+\gamma$ becomes $\ln ka_0$ where a_0 is the Bohr radius. The task is then to determine the unknown functions $\lambda_l(k)$ (in the case of using $\tan\delta_l$) and $\alpha_l(k)$ and $\beta_l(k)$ (in the case of using the Jost function) such that the experimental cross section is well approximated by the "model" cross section $\sigma_1+\sigma_2$. The two methods, based, respectively, on the expansion of $\tan\delta_l$ and on the expansion of the Jost function, will be abbreviated "T" and "J."

Knowledge of the integral cross section alone is in general insufficient to extract the underlying phase shifts unambiguously [45]. However, at sufficiently low collision energies, the p-wave phase shift is determined entirely by the C_4 coefficient, so that it is then possible to extract the s-wave parameters from the integral cross section alone (although the p-wave contribution to the cross section may still be important). In particular the sign of the scattering length can be read off from the slope of the cross section with respect to k.

In a first step, we therefore fixed the p-wave functions as $\lambda_1(k)\equiv 0$, $\alpha_1(k)\equiv 1$, and $\beta_1(k)\equiv 0$, assuming that their precise forms have no influence at low energy. Considering only experimental data for wave numbers smaller than $0.15a_0^{-1}$ and using a total of three free parameters in both methods (T and J), we then fitted the s-wave functions to obtain (in atomic units) for $T3$,

$$\lambda_0(k) = 0.667\,706 - 33.662k^2 - 2038.33k^4, \tag{54}$$

and for $J3$,

$$\alpha_0(k) = 1.0 - 22.2032k^2, \tag{55}$$

$$\beta_0(k) = -0.6651 + 49.8841k^2. \tag{56}$$

Figure 1 shows the experimental cross section (E) together with the model cross sections ($T3$ and $J3$): the experimental cross section is reproduced neatly within the energy range of the fit (but not much beyond). The two methods yield nearly the same value for the scattering length: $T3$ gives $\lambda_0(0) = 0.668a_0$, compared to $0.665a_0$ from $J3$, and 0.56 Å $= 1.1a_0$ from Ref. [47]. Ideally the function $\lambda_0(k)$ deduced from $T3$ would be identical to the ratio $-\beta_0(k)/\alpha_0(k)$ deduced from $J3$: however, at higher energies they start to differ (see Fig. 2), due to the fact that both the expansion for $\tan\delta_l$ and the

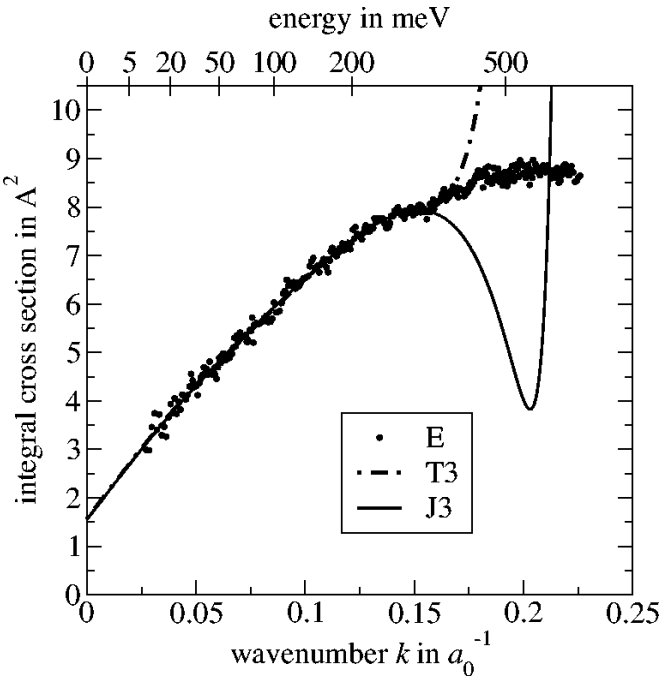

FIG. 1. Comparison of the models $T3$ and $J3$ (see text). E (black dots): the experimental cross section measured by Field *et al.* $J3$ (solid curve) and $T3$ (dotted-dashed curve): cross section obtained by fitting, respectively, the s-wave Jost function ($J3$) and the tangent of the s-wave phase shift ($T3$), using in each method three free parameters and considering only experimental data for $k \leqslant 0.15a_0^{-1}$.

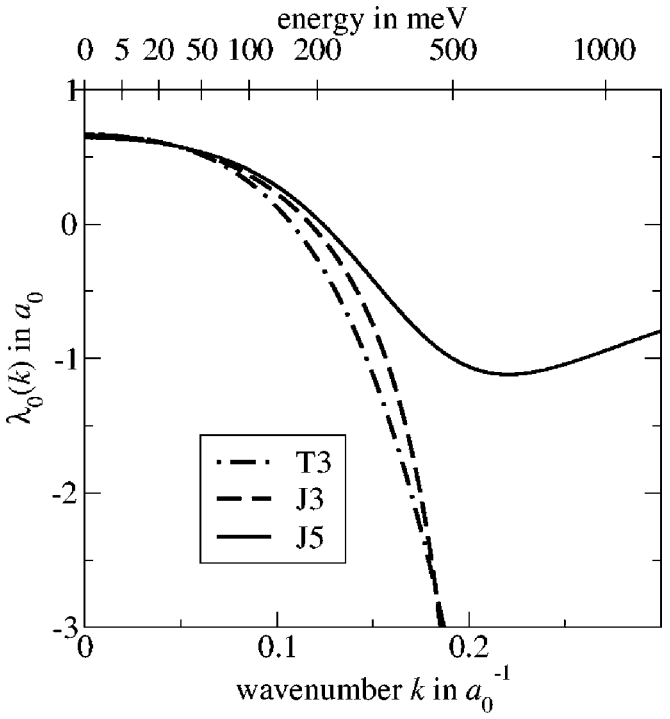

FIG. 2. The fitted function $\lambda_0(k)$ as obtained from $T3$ (dotted-dashed curve), $J3$ (dashed curve), and $J5$ (solid curve). The s-wave scattering length is given by $\lambda_0(0)$.

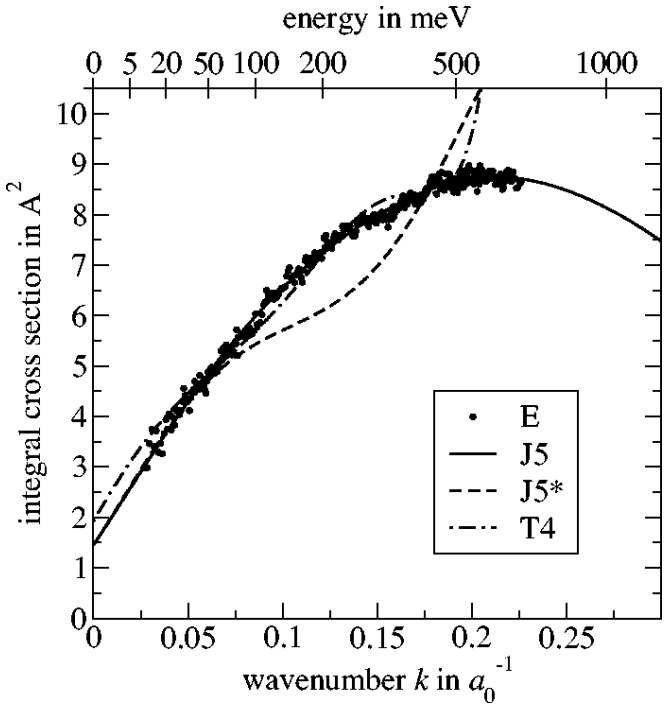

FIG. 3. Fits obtained using higher orders of k. E (black dots): experimental values by Field [46]. $J5$ (solid curve): cross section obtained by fitting both the s-wave and the p-wave Jost function to the experimental data, using a total of five parameters. $J5^\star$ (dashed curve): same as $J5$ but omitting terms of second order in C_4 (see text). $T4$ (dotted-dashed curve): cross section obtained by fitting $\tan\delta_0$ and $\tan\delta_1$ using a total of four free parameters.

expansions for the Jost function are truncated at finite order of C_4k^2.

Next, in an attempt to find out which expansion (T or J) is better suited for interpolating the cross section at higher energies, we increased the number of free parameters from 3 to 5. Using the Jost function we now managed fairly easily, without many trials and errors, to fit $\alpha_l(k)$ and $\beta_l(k)$ ($l=0,1$) such that they reproduce the experimental cross section well in the entire energy range up to 0.7 eV (see Fig. 3). In the five-parameter model $J5$, the fitted functions for the s and p wave are (in atomic units)

$$\alpha_0(k) = 1.0 - 28.0546k^2 + 565.862k^4, \tag{57}$$

$$\beta_0(k) = -0.642\,233 + 41.8624k^2, \tag{58}$$

$$\alpha_1(k) = 1.0, \tag{59}$$

$$\beta_1(k) = -6.12428. \tag{60}$$

The s-wave scattering length deduced from $J5$—that is, the ratio $-\beta_0(0)/\alpha_0(0)=0.64a_0$—is still in fairly good agreement with $J3$ and $T3$. The function $-\beta_0(k)/\alpha_0(k)$ is again plotted in Fig. 2. Certainly the solutions (57)–(60) are not unique: for example, we could have omitted the k^4 term in $\alpha_0(k)$ by adding instead a k^4 correction to $\beta_0(k)$. Therefore we do not attempt to interpret them. Furthermore, it is likely that effects stemming from the anisotropic $1/r^3$ quadrupole and isotropic $1/r^6$ van der Waals interaction would also need to be taken into account in order to determine the "true" parameters.

In Fig. 3 one notices that the curve $J5$ extrapolates smoothly well beyond the range of the experimental data. However, this part of the curve should be regarded with a great deal of skepticism: even if we make the assumption that the influence of higher partial waves and inelastic channels can still be neglected at energies above 0.7 eV, higher orders of k^2 in the s-wave functions $\alpha_0(k)$ and $\beta_0(k)$ could become important, and our theory does not make any prediction on their actual values. Although the expansions allow us to extrapolate the cross section downward in energy, their predictive power for higher energies seems to be rather limited.

While neither of the three-parameter models $J3$ and $T3$ showed any significant advantage over the other, it is interesting that we did not manage to fit the tangent expansion for wave numbers k higher than $\approx 0.18a_0^{-1}$, using trial functions of the form

$$\lambda_0(k) = \lambda_0^{(0)} + \lambda_0^{(1)}k^2 + \lambda_0^{(2)}k^4 + \lambda_0^{(3)}k^6, \tag{61}$$

$$\lambda_1(k) = \lambda_1^{(0)}. \tag{62}$$

Although we tried to adapt the $\lambda_l^{(m)}$ ($m=0,1,2,\ldots$) parameters in a continuous manner, starting at low energies (where the model works), we did not manage to match the model cross section to the experimental one, with or without including the k^6 term in the expression for $\lambda_0(k)$. The curve $T4$ in Fig. 3 shows the model cross section obtained after optimiz-

ing $\lambda_0(k)$ and $\lambda_1(k)$ on the interval $0<k<0.2a_0^{-1}$ using a total of four parameters: clearly it no longer matches the experimental cross section. This failure seems to be related to the appearance of higher orders of $\lambda_0(k)$ in Eq. (50) which contribute very high orders of k: in fact, after truncating Eq. (50) at order k^5 we did manage to fit $\tan\delta_l$ $(l=0,1)$ to the cross section using a total of four parameters. However, since there can be no doubt that the higher orders of k do occur in Eq. (50), we think that they should be retained: the fact that it proved impossible to extend the $T4$ and $T5$ models to higher energies could be seen as an indication that terms of third order in the interaction strength must be included in the expansion of $\tan\delta_l$. Simply omitting the higher orders of k could make the expansion too flexible in the sense that it could then be fitted to rather arbitrary cross sections and would thus be less reliable for extracting scattering lengths and phase shifts or for gathering information about the details of the long-range interactions.

Our conclusion, for this particular experimental integral cross section, is that if all known terms are included in the expansions for both the Jost function and the tangent of the phase shift, the Jost function can still be fitted at energies where the tangent expansion breaks down.

Finally, in order to demonstrate the importance of the second-order terms in the threshold laws (48) and (49) we recalculated the cross section $\sigma_1+\sigma_2$ from the functions $\alpha_l(k)$ and $\beta_l(k)$ $(l=0,1)$ given in Eqs. (57)–(60) by inserting them into (48) and (49) but now *omitting* all terms of order C_4^2: the resulting cross section is represented in Fig. 3, curve $J5^\star$. The deviation of $J5^\star$ from $J5$ shows that second-order effects become important at energies of around 50 meV. Of course the numerical constants in Eqs. (57)–(60) may be readjusted in order to achieve a better agreement of the "first-order cross section" (i.e., the cross section obtained from the Jost function without second-order corrections) and the experimental one. However, we found the first-order Jost function more difficult to fit to the cross section, and we thus conclude that the second-order corrections are not only important from a theoretical point of view but that their presence can also improve the numerical fits.

VI. CONCLUSION

We have derived a simple series in k for the partial-wave Jost function associated with scattering by a central potential that vanishes as $1/r^s$ $(s>2)$: this series is given in Eq. (29). It is a perturbation series reexpanded in k that has been reformulated in such a way that it can now be easily truncated at any desired order in k; it further explains the general structure of modified effective-range expansions for different potentials. Clearly it can be generalized to superpositions of power-law potentials and to coupled partial waves for nonspherical potentials. We have demonstrated its usefulness by rederiving and improving existing expansions for two long-range potentials of particular interest, $s=3$ and $s=4$, in both cases including the contributions which are of second order in the strength of the long-range interaction. In the case of $s=3$, $l=0$ the second-order correction is expected to be important even in the ultralow energy range.

We argued that near-threshold expansions of scattering observables can become simpler when formulated in terms of the Jost function rather than in terms of the phase shift, and for the particular case of scattering of slow electrons on N_2 molecules we showed that the Jost function can be directly fitted (up to a normalizing factor) to the observed cross section.

Further deriving an expansion valid over a large energy range is still a difficult task. An alternative to the effective-range approach makes use of the wave function and its derivative at a fixed distance d where the collision energy is dwarfed by the potential. The wave function and its derivative at d can then be related to asymptotic scattering quantities using energy-dependent analytical [11,16,26,50] or numerical [51–53] solutions of the long-range $1/r^s$ potential. This idea has already been exploited as a starting point of quantum-defect theory [41,42], and it provides another possible approach to the understanding of threshold effects in potential scattering.

In conclusion, the present work proposes a more robust perturbation expansion for potential scattering off structured targets in situations where the isotropic interaction dominates. It has been shown how the use of the Jost function through the formulation of Eq. (29) can lead to a more direct understanding of the role played by the various, potential-linked parameters which include the scattering length and the effective-range parameter.

ACKNOWLEDGMENTS

The financial support of the University of Rome Research Committee and of the EPIC EU network Grant No. HPRN-CT-2002-00179 is gratefully acknowledged. The authors thank E. Bodo for a helpful comment on the paper and T. Stoecklin and J.-M. Launay for stimulating discussions. The authors are also grateful to D. Field for providing his experimental data.

APPENDIX A: CONVERGENCE OF THE PERTURBATION SERIES

In this appendix, the symbol C denotes a constant, though not necessarily the same at each occurrence.

Substitution of Eqs. (13) and (14) for $A_l(k,r)$ and $B_l(k,r)$ in Eq. (8) yields a Volterra equation for the wave function (cf. Chap. 12 of Ref. [38]):

$$u_l(k,r)=u_l^{(0)}(k,r)+k^{-1}\int_d^r dr'\,g_l(kr,kr')V(r')u_l(k,r'), \tag{A1}$$

$$u_l^{(0)}(k,r)=\frac{j_l(kr)}{k^{l+1}}A_l(k,d)-k^l n_l(kr)B_l(k,d), \tag{A2}$$

$$g_l(x,x')=n_l(x)j_l(x')-j_l(x)n_l(x'). \tag{A3}$$

Iteration of (A1) generates the Neumann series

$$u_l(k,r) = \sum_{n=0}^{\infty} u_l^{(n)}(k,r), \tag{A4}$$

$$u_l^{(n)}(k,r) = k^{-n} \int_d^r dr_n \cdots \int_d^{r_2} dr_1 g_l(kr,kr_n) \cdots g_l(kr_2,kr_1) \times V(r_n) \cdots V(r_1) u_l^{(0)}(k,r_1). \tag{A5}$$

Note that $u^{(n)}(k,r)$ in Eq. (A5) is the same as in Eq. (19).

The Riccati-Bessel functions $j_l(x)$ and $n_l(x)$ and the Green's function (A3) are bounded as follows [38]:

$$|j_l(x)| \leqslant C\left(\frac{x}{1+x}\right)^{l+1}, \tag{A6}$$

$$|n_l(x)| \leqslant C\left(\frac{1+x}{x}\right)^{l}. \tag{A7}$$

If $x \leqslant x'$,

$$|g_l(x,x')| \leqslant C\left(\frac{x}{1+x}\right)^{l+1}\left(\frac{x'}{1+x'}\right)^{-l}. \tag{A8}$$

Thus the nth member of the series (A4) is bounded as

$$|u_l^{(n)}(k,r)| \leqslant C^{n+1} \int_d^r dr_n \cdots \int_d^{r_2} dr_1 \left(\frac{r}{1+kr}\right)^{l+1} \times \left(\frac{r_n}{1+kr_n}\right)^{-l} \cdots \left(\frac{r_2}{1+kr_2}\right)^{l+1}\left(\frac{r_1}{1+kr_1}\right)^{-l} \times |V(r_n)| \cdots |V(r_1)| \left(\frac{r_1}{1+kr_1}\right)^{l+1} \tag{A9}$$

$$= C^{n+1}\left(\frac{r}{1+kr}\right)^{l+1} \int_d^r dr_n \cdots \int_d^{r_2} dr_1 \times \frac{r_n}{1+kr_n} \cdots \frac{r_1}{1+kr_1} |V(r_n) \cdots V(r_1)| \tag{A10}$$

$$= C\left(\frac{r}{1+kr}\right)^{l+1} \frac{1}{n!}\left(C\int_d^r dr' \frac{r'}{1+kr'}|V(r')|\right)^n \tag{A11}$$

$$\leqslant C\left(\frac{r}{1+kr}\right)^{l+1} \frac{q^n}{n!}, \tag{A12}$$

where $q = C\int_d^\infty dr' r' |V(r')|$. Using Eqs. (17) and (18) we obtain the following bounds:

$$|A_l^{(n+1)}(k,r)| \leqslant C\frac{q^n}{n!}\int_d^r dr' |V(r')| \frac{r'}{1+kr'} \leqslant C\frac{q^n}{n!}\int_d^\infty dr' |V(r')| r', \tag{A13}$$

$$|B_l^{(n+1)}(k,r)| \leqslant C\frac{q^n}{n!}\int_d^r dr' |V(r')| \left(\frac{r'}{1+kr'}\right)^{2l+2} \leqslant C\frac{q^n}{n!}k^{-2l-2}\int_d^\infty dr' |V(r')|. \tag{A14}$$

Comparing Eqs. (A13) and (A14) to the geometric series shows that $\Sigma_{n=0}^\infty A_l^{(n)}(k,r)$ and $k^{2l+2}\Sigma_{n=0}^\infty B_l^{(n)}(k,r)$ converge uniformly on the open region $\{(k,r): 0 \leqslant k < \infty; d \leqslant r < \infty\}$. Differentiating the series (15) and (16) with respect to r and using Eqs. (17), (18), and (A4) one sees that they satisfy the variable-constant equations (13) and (14).

APPENDIX B: EXPLICIT ANALYSIS FOR $s=3$, $l=0$

The step from (22)–(29) in Sec. III is investigated explicitly here for the specific case of $s=3$, $l=0$. We shall now omit the partial-wave index $l=0$ on all symbols, and we expand the Jost function as

$$A(k,r) = a_0(r) + k^2 a_1(r) + Ok^4, \tag{B1}$$

$$B(k,r) = b_0(r) + k^2 b_1(r) + Ok^4. \tag{B2}$$

1. Long-range behavior

For distances where the potential is $V(r) = C_3/r^3$ the variable-phase equations (13) and (14) take the form

$$\frac{\partial}{\partial r}\begin{bmatrix} A \\ kB \end{bmatrix} = \frac{C_3}{2kr^3}\begin{bmatrix} \sin 2kr & 1+\cos 2kr \\ \cos 2kr - 1 & -\sin 2kr \end{bmatrix}\begin{bmatrix} A \\ kB \end{bmatrix}. \tag{B3}$$

Using the Taylor series for sine and cosine one sees that $a_m(r)$ and $b_m(r)$ $(m=0,1)$, which give $A(k,r)$ and $B(k,r)$ correctly up to and including order k^2, verify the following linear first-order equations:

$$\frac{d}{dr}\begin{bmatrix} a_0 \\ b_0 \end{bmatrix} = C_3\begin{bmatrix} r^{-2} & r^{-3} \\ -r^{-1} & -r^{-2} \end{bmatrix}\begin{bmatrix} a_0 \\ b_0 \end{bmatrix}, \tag{B4}$$

$$\frac{d}{dr}\begin{bmatrix} a_1 \\ b_1 \end{bmatrix} = C_3\begin{bmatrix} -\frac{2}{3} & -r^{-1} \\ \frac{1}{3}r & \frac{2}{3} \end{bmatrix}\begin{bmatrix} a_0 \\ b_0 \end{bmatrix} + C_3\begin{bmatrix} r^{-2} & r^{-3} \\ -r^{-1} & -r^{-2} \end{bmatrix}\begin{bmatrix} a_1 \\ b_1 \end{bmatrix}. \tag{B5}$$

The long-range forms of $a_m(r)$ and $b_m(r)$ $(m=0,1)$ can be determined from these differential equations by making the ansatz

$$\begin{bmatrix} a_m(r) \\ b_m(r) \end{bmatrix} = \begin{bmatrix} \alpha_m \\ \beta_m \end{bmatrix} + \sum_{n=1}^{\infty} C_3^n \begin{bmatrix} a_m^{(n)}(r) \\ b_m^{(n)}(r) \end{bmatrix}. \tag{B6}$$

We thus obtain

$$\begin{bmatrix} a_0(r) \\ b_0(r) \end{bmatrix} = \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix} + C_3 \begin{bmatrix} -r^{-1} & -\frac{1}{2}r^{-2} \\ -\ln\frac{r}{\rho} & r^{-1} \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix} + C_3^2 \begin{bmatrix} \frac{1}{2}r^{-2}\left(\ln\frac{r}{\rho}+\frac{3}{2}\right) & -\frac{1}{6}r^{-3} \\ -r^{-1}\left(\ln\frac{r}{\rho}+2\right) & \frac{1}{4}r^{-2} \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix} + OC_3^3, \tag{B7}$$

$$\begin{bmatrix} a_1(r) \\ b_1(r) \end{bmatrix} = \begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix} + C_3 \begin{bmatrix} -\frac{2}{3}r & -\ln\frac{r}{\rho} \\ \frac{1}{6}r^2 & \frac{2}{3}r \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix} + C_3 \begin{bmatrix} -r^{-1} & -\frac{1}{2}r^{-2} \\ -\ln\frac{r}{\rho} & r^{-1} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix} + C_3^2 \begin{bmatrix} \frac{1}{2}\ln^2\frac{r}{\rho}+\frac{1}{6}\ln\frac{r}{\rho}, & r^{-1}\left(\ln\frac{r}{\rho}+1\right) \\ -\frac{2}{3}r\left(\ln\frac{r}{\rho}-\frac{5}{4}\right), & \frac{1}{2}\ln^2\frac{r}{\rho}-\frac{1}{6}\ln\frac{r}{\rho} \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix}$$
$$+ C_3^2 \begin{bmatrix} \frac{1}{2}r^{-2}\left(\ln\frac{r}{\rho}+\frac{3}{2}\right) & -\frac{1}{6}r^{-3} \\ -r^{-1}\left(\ln\frac{r}{\rho}+2\right) & \frac{1}{4}r^{-2} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix} + OC_3^3. \tag{B8}$$

One sees that in the general case of $\alpha_0 \neq 0$ only $a_0(r)$ remains finite when $r \to \infty$, whereas $b_0(r)$, $a_1(r)$, and $b_1(r)$ diverge. Similarly it can be shown that $a_m(r)$ and $b_m(r)$ $(m=2,3,\ldots)$ generally diverge. Combining Eqs. (B7) and (B8) results in the following long-range form for the r-dependent Jost function [this form can also be derived by iterating Eqs. (B3) using the variable $x=kr$ and replacing $\ln x$ by $\ln(r/\rho)$ in the end]

$$\begin{bmatrix} A(k,r) \\ kB(k,r) \end{bmatrix} = \Bigg\{ 1 + kC_3 \begin{bmatrix} -(kr)^{-1} - \frac{2}{3}kr + O(kr)^3, & -\frac{1}{2}(kr)^{-2} - \ln\frac{r}{\rho} + O(kr)^2 \\ -\ln\frac{r}{\rho} + \frac{1}{6}(kr)^2 + O(kr)^4, & (kr)^{-1} + \frac{2}{3}kr + O(kr)^3 \end{bmatrix}$$
$$+ (kC_3)^2 \begin{bmatrix} \frac{1}{2}(kr)^{-2}\left(\ln\frac{r}{\rho}+\frac{3}{2}\right) + \frac{1}{2}\ln^2\frac{r}{\rho} + \frac{1}{6}\ln\frac{r}{\rho} + O(kr)^2, & -\frac{1}{6}(kr)^{-3} + (kr)^{-1}\left(\ln\frac{r}{\rho}+1\right) + O(kr) \\ -(kr)^{-1}\left(\ln\frac{r}{\rho}+2\right) - \frac{2}{3}kr\left(\ln\frac{r}{\rho}-\frac{5}{4}\right) + O(kr)^3, & +\frac{1}{4}(kr)^{-2} + \frac{1}{2}\ln^2\frac{r}{\rho} - \frac{1}{6}\ln\frac{r}{\rho} + O(kr)^2 \end{bmatrix} + OC_3^3 \Bigg\}$$
$$\times \begin{bmatrix} \alpha_0 + k^2\alpha_1 + Ok^4 \\ k\beta_0 + k^3\beta_1 + Ok^5 \end{bmatrix}. \tag{B9}$$

In Sec. III we pointed out that the long-range functions $\alpha(k)$ and $\beta(k)$ generally depend on the choice made for ρ. However the *form* of Eqs. (B7) and (B8) must, of course, be independent of this choice. In fact it may be checked that Eqs. (B7) and (B8) are invariant under the transformation

$$\rho \to \rho' \tag{B10}$$

$$\alpha_0 \to \alpha_0' = \alpha_0 \tag{B11}$$

$$\beta_0 \to \beta_0' = \beta_0 + C_3 \ln(\rho/\rho')\alpha_0, \tag{B12}$$

$$\alpha_1 \to \alpha_1' = \alpha_1 + C_3 \ln(\rho/\rho')\beta_0 + \tfrac{1}{2}C_3^2 \ln^2(\rho/\rho')\alpha_0 - \tfrac{1}{6}C_3^2 \ln(\rho/\rho')\alpha_0, \tag{B13}$$

$$\beta_1 \to \beta_1' = \beta_1 + C_3 \ln(\rho/\rho')\alpha_1 + \tfrac{1}{2}C_3^2 \ln^2(\rho/\rho')\beta_0 + \tfrac{1}{6}C_3^2 \ln(\rho/\rho')\beta_0 + OC_3^3. \tag{B14}$$

In order to determine the exact transformation law for β_1 it would be necessary to evaluate $b_1(r)$ to third order in C_3.

2. Low-energy expansion

Substituting for $A(k,d)$ and $B(k,d)$ on the right-hand side of (22) the long-range form (B9) with $r=d$, and further expanding $M_1(kd,\infty)$ and $M_2(kd,\infty)$ around $k=0$ (see Appendix D) gives

$$\begin{bmatrix} A(k,\infty) \\ kB(k,\infty) \end{bmatrix} = \left\{ 1 + kC_3 \begin{bmatrix} -\frac{\pi}{2} + x^{-1} + \frac{2}{3}x + Ox^3, & \frac{1}{2}x^{-2} + \ln 2x + \gamma - \frac{3}{2} + Ox^2 \\ \ln 2x + \gamma - \frac{3}{2} - \frac{1}{6}x^2 + Ox^4, & \frac{\pi}{2} - x^{-1} - \frac{2}{3}x + Ox^3 \end{bmatrix} \right.$$
$$+ (kC_3)^2 \begin{bmatrix} Ox^{-1} + \frac{1}{2}\left[\left(\ln 2x + \gamma - \frac{5}{3}\right)^2 + \frac{3}{2} + \frac{\pi^2}{4}\right] + Ox, & Ox^{-1} - \frac{\pi}{2}\left(\ln 2x + \gamma - \frac{4}{3}\right) + Ox \\ Ox^{-1} + \frac{\pi}{2}\left(\ln 2x + \gamma - \frac{5}{3}\right) + Ox, & Ox^{-1} + \frac{1}{2}\left[\left(\ln 2x + \gamma - \frac{4}{3}\right)^2 + \frac{17}{18} + \frac{\pi^2}{4}\right] + Ox \end{bmatrix}$$
$$\left. + OC_3^2 \right\} \times \left\{ 1 + kC_3 \begin{bmatrix} -x^{-1} - \frac{2}{3}x + Ox^3, & -\frac{1}{2}x^{-2} - \ln\frac{x}{k\rho} + Ox^2 \\ -\ln\frac{x}{k\rho} + \frac{1}{6}x^2 + Ox^4, & x^{-1} + \frac{2}{3}x + Ox^3 \end{bmatrix} \right.$$
$$+ (kC_3)^2 \begin{bmatrix} \frac{1}{2}x^{-2}\left(\ln\frac{x}{k\rho} + \frac{3}{2}\right) + \frac{1}{2}\ln^2\frac{x}{k\rho} + \frac{1}{6}\ln\frac{x}{k\rho} + Ox^2 & -\frac{1}{6}x^{-3} + x^{-1}\left(\ln\frac{x}{k\rho} + 1\right) + Ox \\ -x^{-1}\left(\ln\frac{x}{k\rho} + 2\right) - \frac{2}{3}x\left(\ln\frac{x}{k\rho} - \frac{5}{4}\right) + Ox^3, & +\frac{1}{4}x^{-2} + \frac{1}{2}\ln^2\frac{x}{k\rho} - \frac{1}{6}\ln\frac{x}{k\rho} + Ox^2 \end{bmatrix} \left. + OC_3^3 \right\} \begin{bmatrix} \alpha(k) \\ k\beta(k) \end{bmatrix}, \tag{B15}$$

where $x=kd$. The above expression is a special case of (28). Multiplying out the individual terms and retaining only those that are of zero order in d results in Eqs. (44) and (45). Note that the logarithmic terms in Eq. (B15), $\ln(kd)$ and $\ln(d/\rho)$, combine neatly so that $\ln d$ drops out.

3. The special case of $A(0,\infty)=0$

The discrepancy between (44) and (45) and Eq. (3.4b) of Ref. [15] might be explained qualitatively as follows. In the case of $A(k=0,\infty)=\alpha_0=0$, it could be possible that the estimates in Ref. [15] amount to approximating the radial wave function $u(k,r)$ at large distances and for small energies by the long-range form of the zero-energy solution [cf. (B7)],

$$u(k,r) \approx \beta_0 + Ok^2. \tag{B16}$$

Although the approximation (B16) is correct to order k^2 at any large distance r, it is not correct at large distances if k is fixed and positive. In fact, at sufficiently large distances the kinetic energy dominates over the potential, and the true solution oscillates sinusoidally. Nevertheless, let us insert (B16) on the right-hand side of (13) and (14), take the limit for $r\to\infty$ and denote the result $\tilde{A}$ and $\tilde{B}$,

$$\tilde{A}(k,\infty) \equiv A(k,d) + C_3k^2\int_{kd}^{\infty}\frac{\cos t}{t^3}dt(\beta_0 + Ok^2)$$
$$= a_0(d) + C_3\frac{1}{2}\left(k^2\ln k + \frac{1}{d^2}\right)\beta_0 + Ok^2, \tag{B17}$$

$$k\tilde{B}(k,\infty) \equiv kB(k,d) - C_3k^2\int_{kd}^{\infty}\frac{\sin t}{t^3}dt(\beta_0 + Ok^2)$$
$$= kb_0(d) - C_3\frac{k}{d}\beta_0 + Ok^2. \tag{B18}$$

Although these expressions are correct only to first order in C_3, they become exact in the limit $d\to\infty$,

$$\tilde{A}(k,\infty) = C_3(\beta_0/2)k^2\ln k + Ok^2, \tag{B19}$$
$$k\tilde{B}(k,\infty) = \beta_0 k + Ok^2, \tag{B20}$$

which coincides with the result of Eq. (3.4b) in Ref. [15].

However, by repeating the procedure, now using instead of (B16) the better approximation

$$u(k,r) \approx k^{-1}\sin(kr)A(k,d) + \cos(kr)B(k,d), \tag{B21}$$

we obtain

$$\tilde{A}(k,\infty) = C_3\beta_0k^2\ln k + Ok^2, \tag{B22}$$
$$k\tilde{B}(k,\infty) = \beta_0 k + Ok^2, \tag{B23}$$

in accordance with our Eqs. (44) and (45).

Of course the fact that (B16) is not a valid approximation does not imply that the resulting expression (B19) is incorrect. However it suggests that the derivation of Eq. (3.4b) in Ref. [15] should be further checked.

APPENDIX C: EXPLICIT ANALYSIS FOR $s=4$, $l=0$

As in the preceding section, we substitute for $A(k,d)$ and $B(k,d)$ in Eq. (22) their long-range forms and further expand $M_1(kd,\infty)$ and $M_2(kd,\infty)$ around $k=0$, to obtain

$$\begin{bmatrix} A(k,\infty) \\ kB(k,\infty) \end{bmatrix} = \left\{ 1 + kC_4 \begin{bmatrix} \frac{2}{3}\ln 2x + \frac{2}{3}\gamma - \frac{11}{9} + \frac{1}{2}x^{-2} - \frac{1}{15}x^2 + Ox^4, & \frac{\pi}{3} + \frac{1}{3}x^{-3} - x^{-1} - \frac{1}{3}x + Ox^3 \\ \frac{\pi}{3} - x^{-1} - \frac{1}{3}x + Ox^3, & -\frac{2}{3}\ln 2x - \frac{2}{3}\gamma + \frac{11}{9} - \frac{1}{2}x^{-2} + \frac{1}{15}x^2 - Ox^4 \end{bmatrix} \right.$$
$$+ (k^2C_4)^2 \begin{bmatrix} Ox^{-2} + \frac{2}{9}\left[\left(\ln 2x + \gamma - \frac{9}{5}\right)^2 + \frac{163}{100} + \frac{\pi^2}{4}\right] + Ox^2, & Ox^{-3} + Ox^{-1} - \frac{\pi}{2}\left(\ln 2x + \gamma - \frac{28}{15}\right) + Ox \\ Ox^{-1} + \frac{\pi}{2}\left(\ln 2x + \gamma - \frac{9}{5}\right) + Ox, & Ox^{-2} + \frac{2}{9}\left[\left(\ln 2x + \gamma - \frac{28}{15}\right)^2 + \frac{1561}{900} + \frac{\pi^2}{4}\right] + Ox^2 \end{bmatrix}$$
$$\left. + OC_4^2 \right\} \times \left\{ 1 + kC_4 \begin{bmatrix} -\frac{2}{3}\ln 2x - \frac{2}{3}\gamma + \frac{11}{9} - \frac{1}{2}x^{-2} + \frac{1}{15}x^2 - Ox^4, & -\frac{\pi}{3} - \frac{1}{3}x^{-3} + x^{-1} + \frac{1}{3}x - Ox^3 \\ -\frac{\pi}{3} + x^{-1} + \frac{1}{3}x - Ox^3, & +\frac{2}{3}\ln 2x + \frac{2}{3}\gamma - \frac{11}{9} + \frac{1}{2}x^{-2} - \frac{1}{15}x^2 + Ox^4 \end{bmatrix} \right.$$
$$+ (k^2C_4)^2 \begin{bmatrix} Ox^{-2} + \frac{2}{9}ln^2\frac{x}{k\rho} - \frac{2}{135}\ln\frac{x}{k\rho} + Ox^2, & Ox^{-5} \\ Ox^{-3}, & Ox^{-2} + \frac{2}{9}ln^2\frac{x}{k\rho} + \frac{2}{135}\ln\frac{x}{k\rho} + Ox^2 \end{bmatrix}$$
$$\left. + OC_4^3 \right\} \begin{bmatrix} \alpha(k) \\ k\beta(k) \end{bmatrix}, \tag{C1}$$

where $x=kd$. The above expression is again a special case of (28). Multiplying out the individual terms and retaining only those of zero order in d then gives (48) and (49). Again the logarithms $\ln kd$ and $\ln r/\rho$ combine in such a way that $\ln d$ cancels.

APPENDIX D: INTEGRALS

In the case of $l=0$, the Riccati-Bessel functions are $j_0(x)=\sin x$ and $n_0(x)=-\cos x$. In this case the integrals $M_n(x)$ $(n=1,2)$ defined by (23) can be expanded in x using elementary arithmetics: both the simple and the double integrals, $M_1(x)$ and $M_2(x)$, are first related to Si x and Ci x using partial integrations, and their expansions around $x=0$ are then obtained from the known expansions of Si x and Ci x [54]. In the case of the double integrals $M_2(x)$ we have further used the identity

$$\int_0^\infty \frac{\cos t}{t}\mathrm{Si}\, t dt = -\int_0^\infty \frac{\sin t}{t}\mathrm{Ci}\, t dt = 0, \tag{D1}$$

which follows from Eqs. (11.1.1) and (11.4.6) of Ref. [55]. The calculations are rather tedious. In the case of the double integrals we have therefore only evaluated the terms of logarithmic order, which are the only ones that appear in the second-order perturbative correction of the threshold law.

1. $s=3$, $l=0$

In the case of $s=3$, $l=0$, we have

$$M_1(x,\infty) = \int_x^\infty dt t^{-3} \begin{bmatrix} \cos t \sin t & \cos t \cos t \\ -\sin t \sin t & -\sin t \cos t \end{bmatrix}$$
$$= \begin{bmatrix} -\frac{\pi}{2} - 2\sum_{m=0}^\infty \frac{(-1)^m}{(2m+1)!}\frac{(2x)^{2m-1}}{2m-1}, & \ln 2x + \gamma - \frac{3}{2} + \frac{1}{2}x^{-2} + 2\sum_{m=1}^\infty \frac{(-1)^m}{(2m+2)!}\frac{(2x)^{2m}}{2m} \\ \ln 2x + \gamma - \frac{3}{2} + 2\sum_{m=1}^\infty \frac{(-1)^m}{(2m+2)!}\frac{(2x)^{2m}}{2m}, & \frac{\pi}{2} + 2\sum_{m=0}^\infty \frac{(-1)^m}{(2m+1)!}\frac{(2x)^{2m-1}}{2m-1} \end{bmatrix}, \tag{D2}$$

$$M_2(x,\infty) = \int_x^\infty dt t^{-3} \begin{bmatrix} \cos t \sin t & \cos t \cos t \\ -\sin t \sin t & -\sin t \cos t \end{bmatrix} \int_x^t dt' t'^{-3} \begin{bmatrix} \cos t' \sin t' & \cos t' \cos t' \\ -\sin t' \sin t' & -\sin t' \cos t' \end{bmatrix}$$
$$= \begin{bmatrix} Ox^{-2} + \frac{1}{2}\left[\left(\ln 2x + \gamma - \frac{5}{3}\right)^2 + \frac{3}{2} + \frac{\pi^2}{4}\right] + Ox^2, & Ox^{-3} + Ox^{-1} - \frac{\pi}{2}\left(\ln 2x + \gamma - \frac{4}{3}\right) + Ox \\ Ox^{-1} + \frac{\pi}{2}\left(\ln 2x + \gamma - \frac{5}{3}\right) + Ox, & Ox^{-2} + \frac{1}{2}\left[\left(\ln 2x + \gamma - \frac{4}{3}\right)^2 + \frac{17}{18} + \frac{\pi^2}{4}\right] + Ox^2 \end{bmatrix}. \tag{D3}$$

2. $s=4$, $l=0$

In the case of $s=4$, $l=0$, we have

$$M_1(x,\infty) = \int_x^\infty dt t^{-4} \begin{bmatrix} \cos t \sin t & \cos t \cos t \\ -\sin t \sin t & -\sin t \cos t \end{bmatrix}$$
$$= \begin{bmatrix} \frac{2}{3}\ln 2x + \frac{2}{3}\gamma - \frac{11}{9} + \frac{1}{2}x^{-2} + 4\sum_{m=2}^{\infty} \frac{(-1)^m}{(2m+3)!}\frac{(2x)^{2m}}{2m}, & \frac{\pi}{3} + \frac{1}{3}x^{-3} - 4\sum_{m=1}^{\infty} \frac{(-1)^m}{(2m)!}\frac{(2x)^{2m-3}}{2m-3} \\ \frac{\pi}{3} - 4\sum_{m=1}^{\infty} \frac{(-1)^m}{(2m)!}\frac{(2x)^{2m-3}}{2m-3}, & -\frac{2}{3}\ln 2x - \frac{2}{3}\gamma + \frac{11}{9} - \frac{1}{2}x^{-2} - 4\sum_{m=2}^{\infty} \frac{(-1)^m}{(2m+3)!}\frac{(2x)^{2m}}{2m} \end{bmatrix}, \tag{D4}$$

$$M_2(x,\infty) = \int_x^\infty dt t^{-4} \begin{bmatrix} \cos t \sin t & \cos t \cos t \\ -\sin t \sin t & -\sin t \cos t \end{bmatrix} \int_x^t dt' t'^{-4} \begin{bmatrix} \cos t' \sin t' & \cos t' \cos t' \\ -\sin t' \sin t' & -\sin t' \cos t' \end{bmatrix}$$
$$= \begin{bmatrix} Ox^{-2} + \frac{2}{9}\left[\left(\ln 2x + \gamma - \frac{9}{5}\right)^2 + \frac{163}{100} + \frac{\pi^2}{4}\right] + Ox^2, & Ox^{-3} + Ox^{-1} - \frac{\pi}{2}\left(\ln 2x + \gamma - \frac{28}{15}\right) + Ox \\ Ox^{-1} + \frac{\pi}{2}\left(\ln 2x + \gamma - \frac{9}{5}\right) + Ox, & Ox^{-2} + \frac{2}{9}\left[\left(\ln 2x + \gamma - \frac{28}{15}\right)^2 + \frac{1561}{900} + \frac{\pi^2}{4}\right] + Ox^2 \end{bmatrix}. \tag{D5}$$

3. $s=4$, $l \geqslant 1$

In the case of $s=4$, $l \geqslant 1$, the matrix

$$M_1(x) = \int_x^\infty dt t^{-4} \begin{bmatrix} -n_l(t) j_l(t) & n_l(t) n_l(t) \\ -j_l(t) j_l(t) & j_l(t) n_l(t) \end{bmatrix} \tag{D6}$$

can be read off from Eqs. (B2), (B5), and (B7) of Ref. [13], noting that the integrals I, J, and K used by Hinckelmann and Spruch are related to M_1 as

$$C_4 k^3 M_1^{AA}(kd,\infty) = -J, \tag{D7}$$

$$C_4 k^3 M_1^{AB}(kd,\infty) = K - I, \tag{D8}$$

$$C_4 k^3 M_1^{BA}(kd,\infty) = -I, \tag{D9}$$

$$C_4 k^3 M_1^{BB}(kd,\infty) = J. \tag{D10}$$

Hence, for $l \geqslant 1$,

$$L_1^{AA}(x) = -L_1^{BB}(x)$$
$$= -\frac{2\ln 2x + 2\gamma - \sum_{j=0}^{l-1} \frac{4}{2j+1} - \frac{2}{2l+1} + \frac{4l^2+4l+5}{(2l+3)(2l-1)}}{(2l+3)(2l+1)(2l-1)}, \tag{D11}$$

$$L_1^{AB}(x) = L_1^{BA}(x) = -\frac{\pi}{(2l+3)(2l+1)(2l-1)}. \tag{D12}$$

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[57] As a simple example consider expanding the function $f(x)=(1+ax)/(1+bx)$ around $x=0$. While only terms of order x need to be retained in both the nominator and the denominator, higher orders of x are needed in order to represent the function by its Taylor series, except in the special case of $a=b$.