Jost functions and singular attractive potentials

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We use Jost functions to determine the leading and next-to-leading terms of the phase shifts $\delta_l(k)$ in the case of homogeneous attractive singular potentials $-1/r^\alpha$, $\alpha>2$, for arbitrary angular momentum l with incoming boundary conditions at small distances. The Jost solutions are obtained by solving a Volterra equation and a more general ansatz is used to fit the Jost solutions to the WKB waves in the inner region, where the WKB approximation is accurate. A connection between the phase shifts of attractive and repulsive homogeneous singular potentials is presented. Finally, an alternative formulation of the effective range theory for arbitrary l is proposed, where both, the scattering length and the effective range have the dimension of a length. The ratio of effective range and scattering length is then the same for attractive and repulsive potentials.

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I. INTRODUCTION

Technological advances in the recent years have made it possible to construct nanostructures [1,2], which may be used in guiding and trapping of ultracold atoms. In such devices atom-surface interactions play a fundamental role, therefore, understanding such interactions is of great importance. Atom-surface potentials are described by attractive singular potentials and the geometry of the surface plays a crucial role. While the interaction of atoms with a flat wall is described by the attractive van der Waals potential proportional to $-1/r^3$ for small distances and for large distances, when retardation effects become important, by the highly retarded Casimir-Polder potential proportional to $-1/r^4$ [3], the scattering of atoms by a conducting sphere is governed by a $-1/r^6$ potential for small distances and by a $-1/r^7$ potential for large distances [3–5]. As the energy $E=(\hbar k)^2/2m$ of the particle tends to zero, the leading effect for vanishing angular momentum $l=0$ and potentials falling off faster than $1/r^2$ is quantum reflection, which describes the classically forbidden reflection of a particle without a classical turning point. The quantum reflection amplitude R tends to unity for $k\to 0$ and depends only on the potential tail. The modulus of R can be expressed with the help of a threshold length b, $|R| \overset{k\to 0}{\sim} 1-2bk$, while for potentials falling off faster than $1/r^3$ the phase of the reflection amplitude is determined near threshold by the mean scattering length $\bar{a}$, $\arg R \overset{k\to 0}{\sim} \pi-2\bar{a}k$. For homogeneous attractive potentials $\sim 1/r^\alpha$, and for a number of nonhomogeneous tails, analytical expressions of $\bar{a}$ and b are known [6,7]. Quantum reflection has already been observed in the interaction of cold atoms with flat surfaces [8–10] or with pillar structured surfaces [11]. However, in these cases the experiments are only sensitive to the modulus and not to the phase of the reflection amplitude. In [4] we have shown that using a curved surface, e.g., a sphere, instead of a flat wall provides the possibility of extracting the modulus and the phase of the scattering amplitude. The differential cross section $\frac{d\sigma}{d\Omega}=|f(\theta)|^2$ calculated up to and including order $O(E)$ is completely determined by s and p waves and is finite at threshold if the potential falls off faster than $1/r^3$. For homogeneous attractive singular potentials and absorbing boundary conditions at $r=0$ the leading and next-to-leading term of the complex s-wave phase shifts $\delta_0(k)$ have been calculated [12] with the help of an effective range theory for potentials falling off faster than $1/r^5$ for $r\to 0$ by introducing a complex scattering length $\mathcal{A}_0$ and a complex effective range $\mathcal{R}_{\text{eff},0}$,

$$\frac{k}{\tan\,\delta_0(k)} \overset{k\to 0}{\sim} -\frac{1}{\mathcal{A}_0}+\frac{1}{2}\mathcal{R}_{\text{eff},0}k^2, \tag{1}$$

while for $l=1$ the phase shift is proportional to the p-wave scattering length $\mathcal{A}_1$,

$$\tan\,\delta_1(k) \overset{k\to 0}{\sim} -(\mathcal{A}_1 k)^3. \tag{2}$$

Contrary to the case of elastic scattering in repulsive potentials the general behavior of the phase shifts for arbitrary l in attractive potentials is not known. For repulsive singular potentials many different methods exist to determine phase shifts for the radial Schrödinger equation with arbitrary angular momentum l (see, e.g., [13]). For a repulsive potential proportional to $1/r^\alpha$ the leading contributions are connected to α and l by the following expressions [13]: For $\alpha>2l+3$ we obtain $\tan\,\delta_l(k)\sim k^{2l+1}$, for $\alpha<2l+3$, $\tan\,\delta_l(k)\sim k^{\alpha-2}$, and finally for $\alpha=2l+3$, $\tan\,\delta_l(k)\sim k^{2l+1}\ln k$.

In this paper we want to determine phase shifts for attractive singular potentials. For this case, many authors, e.g., [14,15] discuss the problem of defining boundary conditions at $r\to 0$ so that phase shifts are determined unambiguously. We use inward traveling WKB waves for small distances, which describe complete absorption near the surface. For this purpose Jost solutions are calculated and fitted to the WKB waves in the inner region using a matching method described in Sec. II. The Jost solutions were first used by Jost [16] and are defined as the irregular solutions of the radial Schrödinger equation satisfying [17]

$$\lim_{r\to\infty} e^{\mp ikr} f_\pm(k,r) = 1. \tag{3}$$

To determine the Jost solutions several approaches have been proposed [15,18–20]. We use an integral representation based on a Volterra equation to determine an approximate expression for the Jost solution [21]. For repulsive singular potentials the Jost solutions have been calculated by del Giudice *et al.* in [22]. In Sec. III the leading and next-to-leading terms of $\tan \delta_l(k)$ are presented for arbitrary l. The similarities between attractive and repulsive potentials are outlined in Sec. IV. In particular an effective range expansion (1) for arbitrary l can be found in both cases, where the scattering length $\mathcal{A}_l$ and the effective range $\mathcal{R}_{\text{eff},l}$ have the dimension of a length and the ratio $\mathcal{R}_{\text{eff},l}/\mathcal{A}_l$ is a real number.

To avoid misunderstanding we want to mention that real phase shifts for attractive singular potentials and nonabsorbing boundary conditions already have been analyzed and parametrized by various authors [23–25]. In this case both the scattering length and the effective range are real, but their explicit values depend on the particular model that is used to describe the potential at short distances [25–27]. For absorbing boundary conditions we can determine phase shifts for a given attractive singular potential unambiguously and model independently.

II. JOST FUNCTIONS AND THE MATCHING METHOD

The theory of Jost functions and Jost solutions is described in the literature (e.g., [28]). Most of the applications of Jost functions (e.g., [18,20,29]) are restricted to elastic scattering in repulsive potentials where only the regular solution of the radial Schrödinger equation plays a significant role. However, since the Jost solutions are two linear independent solutions of the radial Schrödinger equation

$$\frac{d^2u_l(k,r)}{dr^2} + \left(k^2 - \frac{2m}{\hbar^2}V(r) - \frac{l(l+1)}{r^2}\right)u_l(k,r) = 0, \quad (4)$$

except for $k=0$, and are independent of the boundary conditions at $r=0$, the restriction to the regular solution is not essential and any other solution with arbitrary boundary conditions at $r=0$ can be constructed as a superposition of the Jost solutions. In this case the Jost solutions can be matched at an arbitrary point $r=r_0$ to the boundary conditions of the problem [30–33].

For potentials falling off at least as $1/r^2$ for $r\to\infty$, the asymptotic behavior of the physical solutions of (4) can be described by free waves

$$u_l(k,r) \overset{r\to\infty}{=} A[e^{-ikr} - (-1)^l S_l(k) e^{ikr}], \quad (5)$$

where $S_l(k)$ is the S matrix and is connected to the phase shift $\delta_l(k)$ through the relation

$$S_l(k) = e^{2i\delta_l(k)}; \quad (6)$$

therefore (5) can be written in terms of the Jost solutions (3),

$$u_l(k,r) = A[f_-(k,r) - (-1)^l S_l(k) f_+(k,r)]. \quad (7)$$

If for $r<r_0$ (with an arbitrary, finite r_0) the exact solution $u_l(k,r)$ of (7) is given by some function $u_{l,0}(k,r)$, with the normalization $u_{l,0}(k,r)=0$ and $u_{l,0}^{(l+1)}(k,0)=1$, for attractive singular potentials $u_{l,0}^{(l+1)}(ik,0)=1$, we can use the logarithmic derivative, as long as the derivative of the wave function is continuous, to fit the solutions at $r=r_0$ [30],

$$\left.\frac{u'_{l,0}}{u_{l,0}}\right|_{r=r_0} = \left.\frac{f'_-(k,r) - (-1)^l S_l(k) f'_+(k,r)}{f_-(k,r) - (-1)^l S_l(k) f_+(k,r)}\right|_{r=r_0}. \quad (8)$$

Defining the Jost functions

$$\mathcal{F}_\pm(k) = W(f_\pm(k,r), u_{l,0})|_{r=r_0}, \quad (9)$$

where W stands for the Wronskian determinant, the scattering matrix can thus be written as

$$S_l(k) = (-1)^l \frac{\mathcal{F}_-(k)}{\mathcal{F}_+(k)}. \quad (10)$$

In the case of elastic scattering of s waves by nonsingular potentials the Jost functions are related with the Jost solutions in a simple way,

$$\mathcal{F}_\pm(k) = f_\pm(k,0), \quad (11)$$

and the phase shift can be obtained from the Jost solutions,

$$\tan \delta_0(k) = \frac{\text{Im}[\mathcal{F}_-(k)]}{\text{Re}[\mathcal{F}_-(k)]} = \frac{\text{Im}[f_-(k,0)]}{\text{Re}[f_-(k,0)]}. \quad (12)$$

For $l\neq 0$ Eq. (11) holds no longer, instead we have

$$\mathcal{F}_\pm(k) = (2l+1)\lim_{r\to 0} r^l f_\pm(k,r). \quad (13)$$

In this case a similar expression to (12) can be found,

$$\tan \delta_l(k) = \frac{\text{Im}[e^{i\pi l/2}\mathcal{F}_-(k)]}{\text{Re}[e^{i\pi l/2}\mathcal{F}_-(k)]}. \quad (14)$$

For inelastic scattering, e.g., for absorbing boundary conditions, (12) and (14) are not valid anymore—the S matrix is no longer unitary and the phase shift $\delta_l(k)$ is a complex quantity due to loss of flux. In this case the Wronski determinant must be calculated to determine the Jost function.

A simple analytical example is the square-well potential,

$$V(r) = \begin{cases} -k_0^2 & \text{for } r \le L, \\ 0 & \text{for } r > L. \end{cases} \quad (15)$$

The Jost solutions are given by [18]

$$f_+(k,r) = \left(\frac{q+k}{2q}e^{-i(q-k)L}e^{iqr} + \frac{q-k}{2q}e^{i(q+k)L}e^{-iqr}\right)\Theta(L-r) + e^{ikr}\Theta(r-L), \quad (16)$$

and $f_-(k,r)=f_+^*(k,r)$, with $q^2=k_0^2+k^2$, and $\Theta(x)$ as the step function.

For the case of elastic scattering, Eqs. (10) and (11) lead to

$$S(k) = \frac{(q+k)e^{i(q-k)L} + (q-k)e^{-i(q+k)L}}{(q+k)e^{-i(q-k)L} + (q-k)e^{i(q+k)L}}, \quad (17)$$

and the (real) phase shift is

$$\delta(k) = -kL + \arctan\left(\frac{k}{q}\tan(qL)\right). \quad (18)$$

On the other hand, for absorbing boundary conditions (inward traveling WKB waves),

$$u_0 = \frac{\text{const}}{\sqrt{\hbar q}} e^{-iqr}, \tag{19}$$

the S matrix takes the form

$$S(k) = \frac{q-k}{q+k} e^{-2ikL}. \tag{20}$$

As expected, due to the loss of flux, the S matrix is not unitary and the phase shift

$$\delta(k) = -kL - \frac{i}{2}\ln\left(\frac{q-k}{q+k}\right) \tag{21}$$

is a complex function. These results can be easily verified by solving the Schrödinger equation with the corresponding boundary conditions.

III. JOST FUNCTIONS AND ATTRACTIVE SINGULAR POTENTIALS

Jost functions and Jost solutions have been used to calculate phase shifts in the case of repulsive singular potentials [14,15,22,28–30,34], but not for the treatment of scattering by attractive singular potentials. In the latter case the difficulty arises trying to define unambiguously the boundary conditions at the origin. While in the case of repulsive potentials all but one solution tends to infinity for $r \to 0$ and thus are unphysical, all wave functions tend to zero for $r \to 0$ in attractive potentials. For singular potentials falling off faster than $1/r^2$ in the limit $r \to 0$ the WKB approximation becomes more and more accurate and the solutions always can be written as WKB waves [6],

$$\psi(r) \overset{r\to 0}{=} \frac{A}{\sqrt{p(r)}} \exp\left(\pm \frac{i}{\hbar}\int_{r_0}^{r} p(r')dr'\right), \tag{22}$$

where $p(r) = \sqrt{2m[E - V(r)]}$ is the local classical momentum. This allows us to choose unambiguously one of the solutions, e.g., the inward traveling WKB wave, which describes absorbing boundary conditions [4]. Matching this wave with an appropriate superposition of the Jost solutions leads to the Jost functions, which finally determine the phase shifts $\delta_l(k)$ with the help of (10).

A. Determination of the Jost solution for homogeneous singular potentials

The scattering problem for homogeneous singular repulsive potentials is by now well described in the literature [13,15,30]. The Jost solutions for the associated Schrödinger equation

$$\frac{d^2}{dr^2}u_l(k,r) + \left(k^2 - \frac{g^2}{r^\alpha} - \frac{l(l+1)}{r^2}\right)u_l(k,r) = 0,$$

$$\alpha > 2, \quad g^2 > 0, \tag{23}$$

have been obtained by del Giudice *et al.* [22,34] from the corresponding Volterra equation by using the matching method described above to fit the Jost solution to the regular solution, and in particular, used to describe the near-threshold behavior of the phase shifts.

In this paper we are going to use Jost solutions of attractive singular potentials [$g^2 < 0$ in (23)] and match them to inward traveling WKB waves at small distances. The Jost solutions for this case can be obtained in a similar way as for the case of repulsive potentials [22] and the solution u_l of (23) is given by (7).

With

$$\mu = l + 1/2, \quad q = k^{(\alpha-2)/\alpha} g^{2/\alpha}, \quad \text{and } z = \left(\frac{k}{g}\right)^{2/\alpha} r, \tag{24}$$

Eq. (23) can be written as

$$\left(\frac{d^2}{dz^2} + q^2 - \frac{q^2}{z^\alpha} - \frac{\mu^2 - 1/4}{z^2}\right)u_l(q,z) = 0, \tag{25}$$

while the boundary conditions for $r \to +\infty$ transform to

$$f_\pm(q,z) \overset{qz\to\infty}{\sim} e^{\pm iqz}. \tag{26}$$

These substitutions imply the relation $qz = kr$ and, therefore qz is always real, independent of the sign of g^2. The dimensionless variable $z = r/r_0$, $r_0 = (g/k)^{2/\alpha}$ is chosen in a way that the coefficients of the kinetic and potential energy are equal at the point r_0 in terms of the parameter q^2 [22], which ensures that the approximations of the iterative solutions, one starting from the origin and the other starting from infinity, have the same order [30].

In order to obtain an expansion in q^2 we are going to find an appropriate integral representation which leads to an iterative expansion. For this we define the function

$$\phi_l(q,z) = z^{-1/2} u_l(q,z), \tag{27}$$

which fulfills the differential equation

$$\left[\frac{d^2}{dz^2} + \frac{1}{z}\frac{d}{dz} + \left(q^2 - \frac{q^2}{z^\alpha} - \frac{\mu^2}{z^2}\right)\right]\phi_l(q,z) = 0, \tag{28}$$

and, therefore, the Jost solution $f_-(q,z)$ can be expressed in terms of a solution $\phi_l^{(-)}(q,z)$ of (28),

$$\phi_l^{(-)}(q,z) \overset{qz\to\infty}{=} z^{-1/2} f_-(q,z). \tag{29}$$

The integral representation of $\phi_l^{(-)}(q,z)$ of (28) in terms of the Green's function

$$G(z,z') = \begin{cases} 0 & \text{for } qz' < qz, \\ \dfrac{H_\mu^{(2)}(qz)H_\mu^{(1)}(qz') - H_\mu^{(2)}(qz')H_\mu^{(1)}(qz)}{W(H_\mu^{(1)}(qz'), H_\mu^{(2)}(qz'))} & \text{for } qz' > qz, \end{cases} \tag{30}$$

for the homogeneous differential equation

$$\left[\frac{d^2}{dz^2} + \frac{1}{z}\frac{d}{dz} + \left(q^2 - \frac{\mu^2}{z^2}\right)\right]\phi_l(q,z) = 0, \tag{31}$$

reads as

$$\phi_l^{(-)}(q,z) = \phi_{l,0}^{(-)}(q,z) - \frac{1}{q}\int_{qz}^{\infty} d(qz')G(z,z')V(z')\phi_l^{(-)}(q,z'), \tag{32}$$

where $\phi_{l,0}^{(-)}(q,z)$ fulfills the boundary condition (29) and is given by

$$\phi_{l,0}^{(-)}(q,z) = \left(\frac{1}{2}\pi q\right)^{1/2} \exp\left(-\frac{1}{2}(\mu+1/2)\pi i\right) H_\mu^{(2)}(qz), \tag{33}$$

with $H_n^{(1,2)}$ as the Hankel functions.

Notice that the integration limits in (32) are real numbers, though the variable z is in general complex, e.g., for attractive potentials, and also the arguments of the Green's function are real.

The Volterra equation (32) can be solved iteratively. For $\phi_l^{(-)}(q,z)$,

$$\phi_l^{(-)}(q,z) = \sum_i \phi_{l,i}^{(-)}(q,z), \tag{34}$$

where $\phi_{l,0}^{(-)}(q,z)$ is defined as in (33) and

$$\phi_{l,i}^{(-)}(q,z) = -\frac{1}{q}\int_{qz}^{\infty} d(qz')G(z,z')V(z')\phi_{l,i-1}^{(-)}(q,z'). \tag{35}$$

Indeed, the sum (34) represents a power expansion in q^2 [22].

The first iterative solution $\phi_{l,1}^{(-)}$ can be solved analytically and we obtain

$$\begin{aligned}\phi_l^{(-)}(q,z) \approx \phi_{l,0}^{(-)}(q,z) + \phi_{l,1}^{(-)}(q,z) = -\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{3}{4}\pi i\right) q^{1/2}\Bigg\{ \exp\left(-\frac{1}{2}\mu\pi i\right)\Gamma(\mu)\left(\frac{z}{2}\right)^{-\mu}\Bigg[q^{-\mu} + \frac{1}{4}\left(\frac{\eta^2}{1+\eta\mu}z^{-2/\eta} - \frac{1}{1-\mu}z^2\right)q^{-\mu+2} \\ + \frac{1}{4\sqrt{\pi}}\frac{\Gamma(-1/\eta)\Gamma(\mu-1/\eta)\Gamma(1/\eta+1/2)}{\Gamma(1/\eta+\mu+1)}\exp\left(i\frac{\pi}{\eta}\right)q^{-\mu+2/\eta+2} + \dots\Bigg] + \exp\left(\frac{1}{2}\mu\pi i\right)\Gamma(-\mu)\left(\frac{z}{2}\right)^{\mu} \\ \times\Bigg[q^{\mu} + \frac{1}{4}\left(\frac{\eta^2}{1-\eta\mu}z^{-2/\eta} - \frac{1}{1+\mu}z^2\right)q^{\mu+2} + \frac{1}{4\sqrt{\pi}}\frac{\Gamma(-1/\eta)\Gamma(-\mu-1/\eta)\Gamma(1/\eta+1/2)}{\Gamma(1/\eta-\mu+1)}\exp\left(i\frac{\pi}{\eta}\right)q^{\mu+2/\eta+2} + \cdots\Bigg]\Bigg\},\end{aligned} \tag{36}$$

with $\eta = 2/(\alpha-2)$.

Finally, from (29) we can determine the Jost solutions $f_\pm(q,z)$,

$$f_-(q,z) = z^{1/2}\phi_l^{(-)}(q,z) \quad \text{and} \quad f_-(q,z) = f_+^*(q^*,z). \tag{37}$$

B. Choice of the boundary conditions

After determining an approximate expression for the Jost solution we now must choose the boundary conditions for $r\to 0$. As mentioned above, the WKB approximation (22) becomes increasingly accurate for singular potentials for $r\to 0$ if the potential falls off faster than $1/r^2$ near the origin, independent of the sign of g^2. In our case we choose inward traveling WKB waves which can be written as [35]

$$u_l(q,z) \overset{qz\to 0}{\sim} z^{1/2}z^{1/(2\eta)}e^{-\eta q z^{-1/\eta}} \overset{\text{def}}{=} u_l^{\text{WKB}}(q,z) = z^{1/2}\phi_l^{\text{WKB}}(q,z). \tag{38}$$

This expression differs from the regular solution in [22] only by the fact, that the product $qz^{-1/\eta}$ is a complex quantity while in the regular case it is a real function. An interesting aspect of (28) is its symmetry relation: For a solution $\phi_l^{(-)}(\mu,\eta;q,z)$ of (28), $\phi_l^{(-)}(\eta\mu,1/\eta;\exp(-i\pi/2)\eta q,z^{-1/\eta})$ is again a solution of this equation. This implies the relation

$$\phi_l^{(-)}(\eta\mu,1/\eta;\exp(-i\pi/2)\eta q,z^{-1/\eta}) \overset{qz\to 0}{\sim} (z^{-1/\eta})^{-1/2}\exp(-\eta q z^{-1/\eta}), \tag{39}$$

where the right-hand side corresponds to $\phi_l^{\text{WKB}}(q,z)$ in (38). Overall we must only determine $\phi_l^{(-)}(q,z)$, and $\phi_l^{\text{WKB}}(q,z)$ can be found by this symmetry relation. To calculate the Jost functions $\mathcal{F}_\pm(k)$ we must evaluate the Wronski determinant of the Jost solution and the WKB solution (9); we do not have to take into account all contributions, but only terms proportional to z^{l+1} and z^{-l} since the Wronski determinant (9) is independent of z.

C. Case $l=0$

We start with the simple case $l=0$ that corresponds to $\mu=1/2$. The approximation of the Jost solution and the WKB solution follows from (36) and (37):

$$f_-(q,z) = 1 - izq - \left(\frac{1}{2}z^2 - \frac{1}{(\alpha-1)(\alpha-2)}z^{2-\alpha}\right)q^2 + i\left(\frac{z^3}{6} - \frac{1}{(\alpha-2)(\alpha-3)}z^{3-\alpha}\right)q^3 + 2^{\alpha-2}\Gamma(1-\alpha)\exp\left(i\alpha\frac{\pi}{2}\right)q^\alpha + i2^{\alpha-2}\Gamma(1-\alpha)\exp\left(i\alpha\frac{\pi}{2}\right)zq^{\alpha+1} + \cdots, \quad (40)$$

$$u_0^{\mathrm{WKB}}(q,z) = \frac{\Gamma(1/(\alpha-2))}{\sqrt{\pi}(\alpha-2)^{1/2-1/(\alpha-2)}}zq^{1/2-1/(\alpha-2)} + \frac{\Gamma(-1/(\alpha-2))}{\sqrt{\pi}(\alpha-2)^{1/2+1/(\alpha-2)}}q^{1/2+1/(\alpha-2)} + \frac{\Gamma(1/(\alpha-2))}{\sqrt{\pi}(\alpha-2)^{3/2-1/(\alpha-2)}}\left(\frac{1}{\alpha-3}z^{3-\alpha} - \frac{\alpha-2}{6}z^3\right)q^{5/2-1/(\alpha-2)} + \frac{\Gamma(-1/(\alpha-2))}{\sqrt{\pi}(\alpha-2)^{3/2+1/(\alpha-2)}}\left(\frac{1}{\alpha-1}z^{2-\alpha} - \frac{\alpha-2}{2}z^2\right)q^{5/2+1/(\alpha-2)} + \frac{1}{3}\frac{2^{4/(\alpha-2)}}{(\alpha-2)^{1/2+3/(\alpha-2)}}\frac{\Gamma(-2/(\alpha-2))\Gamma(2/(\alpha-2)+1/2)}{\Gamma(3/(\alpha-2))\sin(\pi/(\alpha-2))}zq^{5/2+3/(\alpha-2)} + \frac{2^{4/(\alpha-2)}}{(\alpha-2)^{1/2+5/(\alpha-2)}}\frac{\Gamma(-2/(\alpha-2))\Gamma(-3/(\alpha-2))\Gamma(2/(\alpha-2)+1/2)}{\Gamma^2(1/(\alpha-2))\sin(\pi/(\alpha-2))}q^{5/2+5/(\alpha-2)} + \cdots. \quad (41)$$

q and k are related through (24). When g^2 is negative, q is a complex quantity. Introducing the length scale β_α of the potential ($g^2 = -\beta_\alpha^{\alpha-2}$), q can be written as

$$q = (k\beta_\alpha)^{(\alpha-2)/\alpha}e^{-i\pi/\alpha}. \quad (42)$$

β_α defines a typical length scale for quantum mechanical effects. The factor $e^{-i\pi/\alpha}$ has its origin in the transformation from the attractive to the repulsive potential, $g^2 \to -g^2$.

Though the expansions (40) and (41) are valid for any $\alpha > 2$, we restrict our treatment to integer values. The expressions for $f_-(q,z)$ and $u_0^{\mathrm{WKB}}(z)$ are well behaved and (10) leads to

$$\tan\,\delta_0(k) \overset{k\to 0}{\sim} \frac{\Gamma(-\nu)}{\Gamma(\nu)}\nu^{2\nu}e^{-i\pi\nu}(k\beta_\alpha) + \frac{\Gamma(-\nu)\Gamma^2(-2\nu)\Gamma(-3\nu)}{\Gamma^2(\nu)\Gamma(-4\nu)}\nu^{1+6\nu}e^{-3i\pi\nu}(k\beta_\alpha)^3 - \frac{\sqrt{\pi}}{4}\frac{\Gamma(-1/2-1/(2\nu))}{\Gamma(1/(2\nu)+1)}(k\beta_\alpha)^{\alpha-2} + O(k^5), \quad (43)$$

with $\nu = 1/(\alpha-2)$.

For the particular critical values $\alpha_{\mathrm{crit}} = 3,4,5$, the expansion (40) and (41) involves Γ functions with negative integer arguments. Nevertheless well-defined results can be obtained for these cases by taking the limit $\alpha \to \alpha_{\mathrm{crit}}$ in (10),

$$\tan\,\delta_0(k) \overset{k\to 0}{\sim} -(k\beta_3)\ln(k\beta_3) - \left(\ln 2 + 3\gamma - \frac{3}{2} - i\pi\right)(k\beta_3) + O((k\beta_3)^2) \quad \text{for} \quad \alpha = 3, \quad (44)$$

$$\tan\,\delta_0(k) \overset{k\to 0}{\sim} i(k\beta_4) - \frac{\pi}{3}(k\beta_4)^2 + \frac{4}{3}i(k\beta_4)^3\,\ln(k\beta_4) + \frac{2\pi}{3}(k\beta_4)^3 + \left(\frac{8}{3}(\gamma + \ln 2) - \frac{28}{9}\right)i(k\beta_4)^3 + O((k\beta_4)^4) \quad \text{for} \quad \alpha = 4, \quad (45)$$

$$\tan\,\delta_0(k) \overset{k\to 0}{\sim} -\left(\frac{1}{3}\right)^{2/3}\frac{\Gamma(2/3)}{\Gamma(4/3)}(k\beta_5)e^{-i\pi/3} + \frac{1}{3}(k\beta_5)^3\,\ln(k\beta_5) - \left(\frac{13}{36} + \frac{\ln 3}{18} - \frac{\ln 2}{3} - \frac{5}{9}\gamma - \frac{\pi}{6\sqrt{3}} + i\frac{\pi}{9}\right)(k\beta_5)^3 + 3^{-7/6}\frac{2\pi^2}{\Gamma^2(1/3)}e^{-4/3i\pi}(k\beta_5)^4 + O((k\beta_5)^5) \quad \text{for} \quad \alpha = 5. \quad (46)$$

These results can be easily checked by numerically solving the Schrödinger equation (23). For instance, the difference $\mathcal{D}(k\beta_5)$ of the numerical solution $\tan\,\delta_{\mathrm{num}}(k)$ and the analytical solution $\tan\,\delta_{\mathrm{ana}}(k)$,

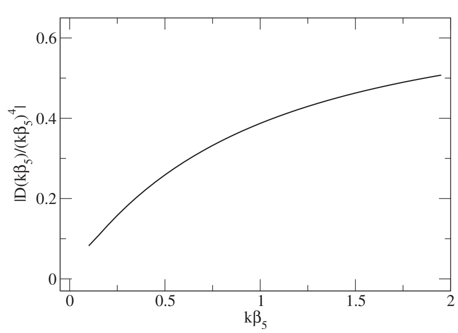

FIG. 1. Comparison between numerical and analytical results for $\alpha = 5$ and $l = 0$ as a function of the dimensionless parameter $k\beta_5$.

$$\mathcal{D}(k\beta_5) = \tan\, \delta_{\mathrm{num}}(k) - \tan\, \delta_{\mathrm{ana}}(k), \tag{47}$$

divided by $(k\beta_5)^4$ is shown in Fig. 1. For $k\beta_5 \to 0$, $|D(k\beta_5)/(k\beta_5)^4|$ tends to 0, therefore, up to order k^4, (46) is correct.

D. Case $l \neq 0$

In this case, the expressions for f_- and u_l^{WKB} can be found in the same way as in the case $l=0$ and are given by

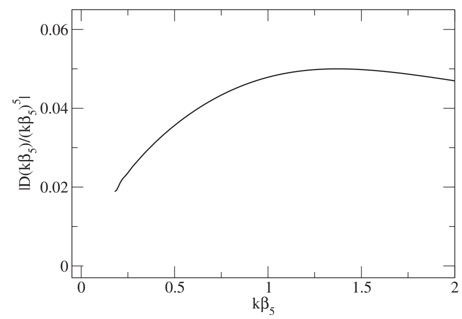

FIG. 2. Comparison between numerical and analytical results for $\alpha=5$ and $l=1$ as a function of the dimensionless parameter $k\beta_5$.

$$f_-(q,z) = -\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{3}{4}\pi i\right)q^{1/2}\Bigg\{\exp\left(-\frac{1}{2}\mu\pi i\right)\Gamma(\mu)2^{\mu}z^{-\mu+1/2}\Bigg[q^{-\mu}+\frac{1}{4}\left(\frac{\eta^2}{1+\eta\mu}z^{-2/\eta}-\frac{1}{1-\mu}z^2\right)q^{-\mu+2}$$
$$+\frac{1}{4\sqrt{\pi}}\frac{\Gamma(-1/\eta)\Gamma(\mu-1/\eta)\Gamma(1/\eta+1/2)}{\Gamma(1/\eta+\mu+1)}\exp\left(i\frac{\pi}{\eta}\right)q^{-\mu+2/\eta+2}+\dots\Bigg]+\exp\left(\frac{1}{2}\mu\pi i\right)\Gamma(-\mu)2^{-\mu}z^{\mu+1/2}$$
$$\times\Bigg[q^{\mu}+\frac{1}{4}\left(\frac{\eta^2}{1-\eta\mu}z^{-2/\eta}-\frac{1}{1+\mu}z^2\right)q^{\mu+2}+\frac{1}{4\sqrt{\pi}}\frac{\Gamma(-1/\eta)\Gamma(-\mu-1/\eta)\Gamma(1/\eta+1/2)}{\Gamma(1/\eta-\mu+1)}\exp\left(i\frac{\pi}{\eta}\right)q^{\mu+2/\eta+2}+\dots\Bigg]\Bigg\} \tag{48}$$

and

$$u_l^{\mathrm{WKB}}(q,z) = \frac{1}{\sqrt{2\pi}}(\eta q)^{1/2}\Bigg\{\Gamma(\eta\mu)2^{\eta\mu}z^{\mu+1/2}\Bigg[(\eta q)^{-\eta\mu}-\frac{1}{4}\left(\frac{1}{\eta^2(\mu+1)}z^2-\frac{1}{1-\eta\mu}z^{-2/\eta}\right)(\eta q)^{-\eta\mu+2}$$
$$-\frac{1}{4\sqrt{\pi}}\frac{\Gamma(-\eta)\Gamma(\eta\mu-\eta)\Gamma(\eta+1/2)}{\Gamma(\eta+\eta\mu+1)}(\eta q)^{-\eta\mu+2\eta+2}+\cdots\Bigg]+\Gamma(-\eta\mu)2^{-\eta\mu}z^{-\mu+1/2}$$
$$\times\Bigg[(\eta q)^{\eta\mu}-\frac{1}{4}\left(\frac{1}{\eta^2(1-\mu)}z^2-\frac{1}{\eta\mu+1}z^{-2/\eta}\right)(\eta q)^{\eta\mu+2}-\frac{1}{4\sqrt{\pi}}\frac{\Gamma(-\eta)\Gamma(-\eta\mu-\eta)\Gamma(\eta+1/2)}{\Gamma(\eta-\eta\mu+1)}(\eta q)^{\eta\mu+2+2\eta}+\cdots\Bigg]\Bigg\}. \tag{49}$$

As for $l=0$ we must distinguish between noncritical cases and the critical cases $\alpha_{\mathrm{crit}}=2l+3$ and $\alpha_{\mathrm{crit}}=2l+5$, where again negative integer arguments in Γ functions appear.

For the noncritical cases we get

$$\tan\, \delta_l(k) \overset{k\to 0}{\sim} \frac{\sqrt{\pi}}{4}\frac{\Gamma(l-1/(2\nu)+1/2)\Gamma(1/(2\nu)+1/2)}{\Gamma(l+1/(2\nu)+3/2)\Gamma(1/(2\nu)+1)}(k\beta_\alpha)^{\alpha-2}-(-1)^l\nu^{2\nu(2l+1)}\frac{\Gamma(-l-1/2)\Gamma(-(2l+1)\nu)}{2^{2l+1}\Gamma(l+1/2)\Gamma((2l+1)\nu)}(k\beta_\alpha)^{2l+1}$$
$$\times e^{-i\pi(2l+1)\nu}-(-1)^l\frac{\sqrt{\pi}\Gamma(-l-1/2)}{2^{2l}\Gamma(l+1/2)}\nu^{2\nu(2l+3)+1}\frac{2^{4\nu}}{2l+1}\frac{\Gamma(-2\nu)}{\Gamma(-2\nu+1/2)}\frac{\Gamma(-(2l+3)\nu)\Gamma((2l-1)\nu)}{\Gamma^2((2l+1)\nu)}(k\beta)^{2l+3}$$
$$\times e^{-i\pi(2l+3)\nu}+O((k\beta_\alpha)^{\rho}), \tag{50}$$

where ρ is an integer number that depends on α and l, $\rho=2(\alpha-2)$ for $l=1, \alpha<9/2+l$, $\rho=2l+5$ for $l=1, \alpha>9/2+l$, $\rho=2(\alpha-2)$ for $l=2,3,\dots,\alpha<6$, $\rho=\alpha+2$ for $l=2,3,\dots,6<\alpha<2l+3$, and $\rho=2l+5$ for $l=2,3,\dots$ and $\alpha>2l+3$.

In the critical cases α_{crit} we again must take the limit $\alpha\to\alpha_{\mathrm{crit}}$ in (10). For $\alpha_{\mathrm{crit}}=2l+3$ we obtain

$$\tan\,\delta_l(k) \overset{k\to 0}{\sim} -\frac{\pi}{2^{2l+2}}\frac{1}{\Gamma^2((2l+3)/2)}(k\beta_{2l+3})^{2l+1}\,\ln(k\beta_{2l+3}) - \frac{\pi}{2^{2l+2}}\frac{1}{\Gamma^2((2l+3)/2)} \times\left[-\frac{i\pi}{2l+1} - \ln 2 - \frac{2}{2l+1}\ln(2l+1) + \frac{1}{2}\Psi(2l+2) - \Psi\left(\frac{2l+3}{2}\right) + \left(\frac{1}{2}+\frac{2}{2l+1}\right)\gamma\right](k\beta_{2l+3})^{2l+1} - (-1)^l\frac{\sqrt{\pi}\Gamma(-l-1/2)}{2^{2l}\Gamma(l+1/2)}(2l+1)^{-4(2l+2)/(2l+1)}2^{4/(2l+1)} \times\frac{\Gamma(-2/(2l+1))}{\Gamma(-2/(2l+1)+1/2)}\Gamma\left(-\frac{2l+3}{2l+1}\right)\Gamma\left(\frac{2l-1}{2l+1}\right)(k\beta_{2l+3})^{2l+3}e^{-i\pi(2l+3)/(2l+1)} + O((k\beta_\alpha)^\rho), \quad (51)$$

with $\rho=2(2l+1)$ for $l=1$ and $\rho=2l+5$ for $l=2,3,4,\ldots$.

For $\alpha_{\text{crit}}=2l+5$ the phase shifts read as

$$\tan\,\delta_l(k) \overset{k\to 0}{\sim} -(-1)^l(2l+3)^{-2(2l+1)/(2l+3)}\frac{\Gamma(-l-1/2)}{2^{2l+1}\Gamma(l+1/2)}\frac{\Gamma(-(2l+1)/(2l+3))}{\Gamma((2l+1)/(2l+3))}(k\beta_{2l+5})^{2l+1}e^{-i\pi(2l+1)/(2l+3)} - \frac{1}{[(2l+3)\,!\,!]^2} \times\Bigg[(2l+3)\ln 2 + 2\ln(2l+3) - \frac{2l+3}{2}\Psi(2l+3) + (2l+3)\Psi\left(\frac{2l+3}{2}\right) + 2\Psi\left(-\frac{2}{2l+3}\right) - \Psi\left(-\frac{4}{2l+3}\right) + \frac{2l+5}{2}\Psi(1) + i\pi - \frac{2l-1}{4}\Bigg](k\beta_{2l+5})^{2l+3} + \frac{2l+3}{[(2l+3)\,!\,!]^2}(k\beta_{2l+5})^{2l+3}\,\ln(k\beta_{2l+5}) + O((k\beta_{2l+5})^{2l+5}), \quad (52)$$

where Ψ stands for the logarithmic derivative of the Γ function and γ is the Euler-Mascheroni constant.

As in the case of $l=0$ we have checked the analytical results numerically. Figure 2 shows the same as Fig. 1 but for $\alpha=5$ and $l=1$. In this case $\mathcal{D}(k\beta_5)$ is divided by k^5.

IV. ATTRACTIVE VERSUS REPULSIVE HOMOGENEOUS SINGULAR POTENTIALS

In [12] we found a simple connection between the s-wave effective range theory for repulsive and attractive homogeneous singular potentials. The transformation $\beta_\alpha \to \beta_\alpha e^{i\pi\nu}$ [i.e., $V_{\text{att}}(r)\to V_{\text{rep}}(r)=-V_{\text{att}}(r)$] and the use of WKB waves for small distances r leads to the relation $\mathcal{A}_0=a_0e^{-i\pi\nu}$ and $\mathcal{R}_{\text{eff},0}=r_{\text{eff},0}e^{-i\pi\nu}$ between the (real) scattering length a_0 and the (real) effective range $r_{\text{eff},0}$ of the repulsive case, and the complex scattering length $\mathcal{A}_0$ and a complex effective range $\mathcal{R}_{\text{eff},0}$ of the attractive case. This property of s-wave scattering is indeed a general feature of homogeneous potentials. As mentioned above, the regular and WKB solution differ only by the fact that in (24) z is a real number for repulsive potentials ($g^2>0$), while it is a complex quantity for attractive potentials ($g^2<0$). However, since the Jost solutions depend only on the product $qz=kr$, which is a real expression and independent of the sign of g^2, and the Jost functions can be expressed by $k\beta_\alpha$ (remember $g^2=\pm\beta_\alpha^{\alpha-2}$), the phase shifts obtained for elastic scattering are also valid in the attractive case where β_α is replaced by $\beta_\alpha e^{-i\pi\nu}$. This implies that the leading contributions (50)–(52) of $\delta_l(k)$ can be obtained through the latter transformation from the phase shifts of repulsive homogeneous potentials given in [22,34]. Moreover, it is possible to define an effective range expansion for arbitrary l for attractive potentials. For repulsive potentials Blatt and Jackson have shown [36] that a scattering length a_l can be defined for potentials falling off faster than $1/r^{2l+3}$ and an effective range $r_{\text{eff},l}$ for potentials falling off faster than $1/r^{2l+5}$. In that case the leading and next-to-leading terms of the phase shift are given by

$$k^{2l+1}\cot[\delta_l(k)] = -\frac{1}{a_l^{2l+1}} + \frac{1}{2}r_{\text{eff},l}^{1-2l}k^2 + O(k^4), \quad (53)$$

which reduces to the ordinary s-wave effective range expansion for $l=0$ [37]. Notice that a_l and $r_{\text{eff},l}$ have the dimension of a length in contrast with the definition used in [28,38].

In a similar way it is possible to find an effective range expansion for $l\geq 0$ for attractive singular potentials with absorbing boundary conditions. In this case (53) preserves its form,

$$k^{2l+1}\cot[\delta_l(k)] = -\frac{1}{\mathcal{A}_l^{2l+1}} + \frac{1}{2}\mathcal{R}_{\text{eff},l}^{1-2l}k^2 + O(k^4), \quad (54)$$

however, as for s waves, the scattering length $\mathcal{A}_l$ and the effective range $\mathcal{R}_{\text{eff},l}$ are complex. For homogeneous repulsive potentials the scattering length a_l and the effective range $r_{\text{eff},l}$ are real. Their analytical expressions read as

$$a_l = \frac{(-1)^l}{2}\nu^{2\nu}\left(\frac{\Gamma(-1/2-l)\Gamma(-(1+2l)\nu)}{\Gamma(l+1/2)\Gamma((1+2l)\nu)}\right)^{1/(2l+1)}\beta_\alpha \quad (55)$$

and

$$r_{\mathrm{eff},l}=\frac{(-1)^l\nu^{2\nu}}{2}\left(\frac{2^{2(1+2\nu)}\sqrt{\pi}\Gamma(1/2+l)\Gamma(1-2\nu)\Gamma((-1+2l)\nu)\Gamma(-(3+2l)\nu)}{\Gamma(1/2-l)\Gamma(1/2-2\nu)\Gamma^2(-(1+2l)\nu)}\right)^{1/(1-2l)}\beta_\alpha, \tag{56}$$

respectively.

For homogeneous attractive potentials $\mathcal{A}_l$ and $\mathcal{R}_{\mathrm{eff},l}$ are connected with the results of the repulsive case by

$$\mathcal{A}_l=a_le^{-i\pi\nu} \quad \text{and} \quad \mathcal{R}_{\mathrm{eff},l}=r_{\mathrm{eff},l}e^{-i\pi\nu}, \tag{57}$$

and again the ratio $\mathcal{R}_{\mathrm{eff},l}/\mathcal{A}_l=r_{\mathrm{eff},l}/a_l$ is a real number.

Note that the last term in (46) is given incorrectly in Eq. (12′) in [22], and some mistakes can be found in Eq. (8) in [34] for $\alpha_{\mathrm{crit}}=2l+5$.

V. CONCLUSION

We calculated the phase shifts $\delta_l(k)$ for attractive singular potentials $\sim 1/r^\alpha$, $\alpha>2$ with the help of Jost solutions. The difficulty of defining phase shifts was solved by choosing incoming boundary conditions for $r\to 0$ and adapting the matching method in the inner region. For an angular momentum $l=0$ the results found by adapting the effective range theory to the case of attractive singular potentials are confirmed. For angular momenta $l\neq 0$ we derived an asymptotic expression for the leading and next-to-leading term for the phase shifts for all $\alpha>2$ and any angular momentum. The solutions for repulsive and attractive homogeneous potentials are connected by a simple relation not only in the case of $l=0$ [12] but also for arbitrary l. When the scattering length and the effective range are defined to have the dimension of a length, also for $l\neq 0$, then their ratio remains real for homogeneous attractive tails.

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