Threshold Law for Attractive Inverse-Cube Interactions

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(Received 7 March 2013; published 24 June 2013)

For scattering by potentials with attractive inverse-cube ($-C_3/r^3$) tails, the threshold law for elastic collisions is presented. The expansion of the scattering phase shift contains all terms up to and including $O(k^2)$ and only relies on the value of the threshold quantum number's remainder $\Delta \in [0, 1)$, which accounts for short-range deviations of the full potential from the pure $-C_3/r^3$ form. In contrast to previous approaches, the threshold law presented provides a connection to the regular solution at zero energy as well as to the position of a weakly bound s-wave state.

DOI: 10.1103/PhysRevLett.110.260401 PACS numbers: 03.65.Nk, 34.20.Cf, 34.50.Cx

Introduction.—We consider elastic collisions in the presence of isotropic interaction potentials that exhibit an attractive inverse-cube long-range behavior $-C_3/r^3$. Such potential tails are generally attributed to an underlying dipole-dipole interaction. The interaction energy between two permanent dipoles, for instance, is described by the inverse-cube law in an anisotropic form. In the absence of permanent dipole moments, the dipole-dipole interaction operator also gives a nonvanishing first-order contribution to the interaction energy when the two colliding partners are alike but in different internal states that are connected via a dipole transition [1]. This kind of interaction is isotropic; it can, in principle, be either attractive or repulsive and might—at large distances—be modified due to retardation effects [2,3]. The nonretarded interaction energy between a neutral, polarizable particle and a conducting wall is also characterized by the long-range $-C_3/r^3$ behavior [4].

Both repulsive and attractive inverse-cube interactions exhibit unique scattering properties. The leading term of the effective-range expansion [5,6] for scattering by potentials that fall off faster than $1/r^3$ is generally characterized by a single parameter, i.e., the scattering length a [7]. It is manifest in the regular radial s-wave solution at zero energy, which is, beyond the interaction region, proportional to $(1 - r/a)$. The need for modifications of the conventional effective-range expansion in the presence of long-range potentials was pointed out by Spruch, O'Malley, and Rosenberg [8]. It turns out that the long-range character of inverse-cube interactions precludes the existence of a finite scattering length. A connection of the low-energy scattering properties to the zero-energy solution has not been established so far.

For elastic collisions in the presence of a repulsive $+C_3/r^3$ interaction, the threshold law was first given by Del Giudice and Galzenati in 1965 [9] and rederived from exact solutions later by Gao [10]. As argued in Ref. [10], the near-threshold behavior of the phase shift for the repulsive case is essentially insensitive to the short-range part of the potential. However, quite the contrary is the case for potentials that are asymptotically attractive. Because of its distinct singularity at the origin, the attractive $-1/r^3$ potential alone does not support the existence of wave functions that are suitable for the description of elastic scattering. Only the deviation of the full potential from the singular $-1/r^3$ form at short distances, i.e., the existence of a repulsive core, enables elastic scattering processes. The short-range part of the interaction potential explicitly needs to be taken into account and has a crucial influence on the collision process at low energies.

For attractive inverse-cube potential tails, the leading-order term of the s-wave scattering phase shift was first derived by Levy and Keller [11],

$$\tan\delta_0 = -\ln(k\beta_3)(k\beta_3) + O(k), \tag{1}$$

where the length β_3 is associated with the asymptotic $-C_3/r^3$ form of the potential [see definition just below Eq. (2)]. This simple formula (1) is widely known [12–15] and offers a correct parametrization of the phase shift in the immediate near-threshold regime. It does, however, neglect all further terms of the order k that contribute to the elastic cross section in the limit of small collision energies and depend on the interaction potential at short distances. These additional terms were first brought to attention in the works of Shakeshaft [16] and Ganas [17], who extended the work of Hinckelmann and Spruch [18] to attractive inverse-cube potentials. Their results, however, depend on the characteristics of a truncated finite-range potential, which is purely artificial (see discussion in Ref. [18]).

In the present work, a general, analytical formula [Eq. (7)] for the low-energy behavior of the scattering phase shift in the presence of an attractive inverse-cube tail potential is derived. The leading-order energy dependence is adopted from the properties of quantum reflection that account for the influence of the pure $-1/r^3$ potential and is explicitly related to the asymptotic form of the regular solution at zero energy. This low-energy expansion depends on only a single parameter, which can be identified with the threshold quantum number's remainder

$\Delta \in [0, 1)$ accounting for the deviation of the full potential from the pure singular $-1/r^3$ form at short distances. A connection to the position of a weakly bound state is established and the contribution of higher partial waves to the low-energy scattering cross section is investigated.

Derivation of the threshold law.—The dimensionless Schrödinger equation for the radial wave function in the potential $-C_3/r^3$ is given by

$$\left[-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} - \frac{1}{\rho^3} - \frac{E}{\mathcal{E}_3}\right]u_l(\rho) = 0, \qquad (2)$$

where all lengths are expressed in terms of the quantal length scale $\beta_3 = 2\mu C_3/\hbar^2$, such that $\rho = r/\beta_3$. The energy $E = \hbar^2 k^2/(2\mu)$ enters Eq. (2) in units of the characteristic energy scale $\mathcal{E}_3 = \hbar^2/(2\mu\beta_3^2)$ associated with the tail potential $-C_3/r^3$.

While at finite energies the solutions of the radial Schrödinger equation (2) cannot be represented in a simple closed analytical form [19], the s-wave solutions at zero energy ($E = 0$) can simply be expressed in terms of Bessel functions: $\sqrt{\rho}J_1(2/\sqrt{\rho})$ and $\sqrt{\rho}Y_1(2/\sqrt{\rho})$. In order to support an elastic scattering process, the full potential $V(r)$ deviates from the singular form of its inverse-cube tail at small distances. Beyond the range of these deviations, where $V(r) \approx -C_3/r^3$, the regular zero-energy solution $u_0(\rho)$ in the full potential $V(r)$ can be expressed as a linear combination of the two solutions in the reference potential $-C_3/r^3$,

$$u_0(\rho) \propto \sqrt{\rho}\left[J_1\left(\frac{2}{\sqrt{\rho}}\right) + \tan(\pi\Delta)Y_1\left(\frac{2}{\sqrt{\rho}}\right)\right]. \qquad (3)$$

This linear combination is determined by the noninteger remainder $\Delta \in [0, 1)$ of the threshold quantum number, which is defined as $n_{\rm th} = n_{\rm max} + \Delta$. It is the hypothetical quantum number at exactly $E = 0$ and is a property of the full potential $V(r)$. The integer $n_{\rm max}$ is the quantum number of the least bound state and is related to the total number of bound states N [number of nodes in $u_0(\rho)$] via $n_{\rm max} = N - 1$.

Assuming that the full interaction potential $V(r)$ is known in all of coordinate space, the threshold quantum number can be estimated via

$$n_{\rm th} \approx \frac{1}{\pi\hbar}\int_{r_{\rm in}}^{\infty}\sqrt{-2\mu V(r)}dr - \frac{\phi_{\rm in}(0)}{2\pi} - \frac{\phi_{\rm out}(0)}{2\pi}, \qquad (4)$$

where the semiclassical Bohr-Sommerfeld quantization rule is corrected by including the appropriate reflection phases (see, e.g., Refs. [20,21]). In the case of an inverse-cube tail potential, the threshold value of the outer reflection phase is given by $\phi_{\rm out}(0) = 3\pi/2$, whereas the inner reflection phase depends on the peculiarities of the short-range potential; for a potential with a singular repulsive inner core, it is well approximated by $\phi_{\rm in} \approx \pi/2$.

Potentials that fall off faster than $-1/r^2$ asymptotically and are more singular than $-1/r^2$ do, in general, support the process of quantum reflection [22]. The complex amplitude R for reflection is connected to the complex $\mathcal{K}$ matrix of the quantum reflection process via the relation $\mathcal{K} = i(1 + R)/(1 - R)$. Considering scattering by the full potential $V(r)$ that deviates from this singular attractive form of its tail at short distances, the low-energy expansion for the phase shift can very generally be given by

$$\tan\delta_0 = \mathrm{Re}(\mathcal{K}) - \mathrm{Im}(\mathcal{K})[\cot(\pi\Delta) + O(k^2)], \qquad (5)$$

using the results of Ref. [23]. For potentials that fall off faster than $-1/r^3$, this relation yields $\tan\delta_0 = -ak + O(k^2)$, with the scattering length given by $a = \bar{a} + b/\tan(\pi\Delta)$ involving the mean scattering length $\bar{a}$ and the threshold length b [21] that depend solely on the singular reference potential; see also Ref. [24]

For the quantum reflection process in a singular attractive potential $-C_3/r^3$, the low-energy limit of the $\mathcal{K}$ matrix is given by

$$\mathcal{K} = -\left[\ln(2k\beta_3) + 3\gamma - \frac{3}{2} - i\pi\right](k\beta_3) + \pi\left[\ln(2k\beta_3) + 3\gamma - \frac{19}{12} - i\pi\right](k\beta_3)^2 + O(k^3), \qquad (6)$$

where $\gamma = 0.577\,215\,66\ldots$ is Euler's constant. In order to obtain Eq. (6), the corresponding formula from Ref. [25] was extended to second order in the wave number k using the result of Willner and Gianturco [26]. With the $\mathcal{K}$ matrix (6), relation (5) yields the main result of this Letter,

$$\tan\delta_0 = -\left[\ln(k\beta_3) + \frac{\pi}{\tan(\pi\Delta)} + 3\gamma + \ln 2 - \frac{3}{2}\right](k\beta_3) + \pi\left[\ln(k\beta_3) + \frac{\pi}{\tan(\pi\Delta)} + 3\gamma + \ln 2 - \frac{19}{12}\right](k\beta_3)^2 + O(k^3), \qquad (7)$$

which is the threshold law for elastic s-wave scattering by potentials with attractive inverse-cube tails and contains all terms up to and including $O(k^2)$. These terms depend (apart from β_3) only on the value of the threshold quantum number's remainder Δ which determines the asymptotic form of the regular solution (3). As for potentials that fall off faster than $-1/r^3$, the phase shift tends to zero in the limit of $k \to 0$; however, a finite value cannot be assigned

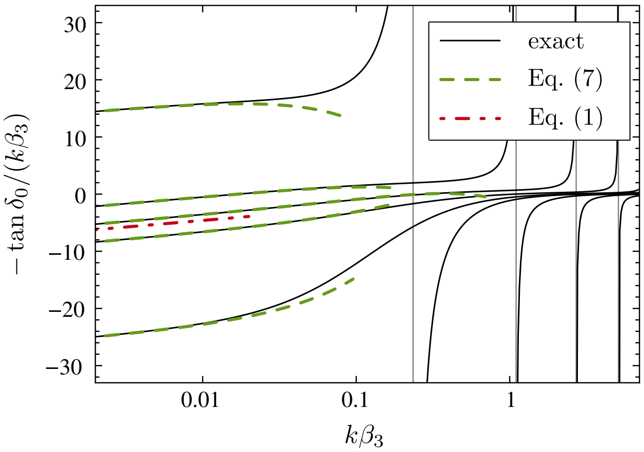

FIG. 1 (color online). The s-wave scattering phase shift for different values of the threshold quantum number's remainder $\Delta = \{0.05, 0.25, 0.5, 0.75, 0.95\}$ (from top to bottom in the limit of low energies). The solid lines show the exact values of $-\tan\delta_0/k$ as a function of the dimensionless product $k\beta_3$. The corresponding results from Eq. (7) are given as dashed lines. They give the correct low-energy behavior. The simple leading-order expansion (1) is depicted by the dot-dashed line.

to the scattering length due to the divergence of the logarithmic term [cf. Eq. (1)].

The result for the special case treated in Refs. [16,17] is retrieved from Eq. (7) by matching the asymptotic form (3) of the regular solution to $(1 - r/a_{sr})$ at the cutoff distance d and keeping only the lowest-order terms in β_3. The present result (7) is, by construction, also compatible with the result of Ref. [26].

Figure 1 shows a plot of the quantity $-\tan\delta_0/k$ against the wave number k in units of $1/\beta_3$. This quantity is sometimes referred to as the energy dependent "effective scattering length" $a_{\text{eff}}(k)$ [27]. It mediates the effective interactions at all collision energies. The solid lines show the exact behavior of $-\tan\delta_0/k$ for five different values of the threshold quantum number's remainder $\Delta = \{0.05, 0.25, 0.5, 0.75, 0.95\}$. These results are obtained from numerically solving the Schrödinger equation (2) with the energy-insensitive inner boundary conditions implied by Eq. (3) and matching to $\sin(kr) + \tan\delta_0\cos(kr)$ at large distances, where the influence of the potential is negligible. The dashed lines in Fig. 1 depict the results obtained from Eq. (7), which—with the given value of the remainder—reproduce the exact results in the low-energy limit. The dot-dashed line shows the crude approximation (1) that contains only the logarithmic term and neglects further terms of $O(k)$.

Presence of a weakly bound state.—For potentials that fall off faster than $-1/r^3$, the magnitude of a large positive scattering length $a > 0$ can be related to the position of a weakly bound state at $E_b = -\hbar^2\kappa_b^2/(2\mu)$ via the relation $a = \kappa_b^{-1} + O(\kappa_b^0)$. A formula that connects the threshold law (7) to the position of a weakly bound state can also be derived in the case of an interaction potential $V(r)$ that behaves as $-C_3/r^3$ at large distances and thus cannot be assigned a finite value for the scattering length.

The highest bound state at the energy $E_b = E_{n_{\max}}$ in the potential well is connected to the threshold quantum number's remainder Δ via the quantization function [20]

$$\Delta = F(E_b) = \kappa_b\beta_3 + O(\kappa_b^2). \tag{8}$$

When the energy E_b is very close to the dissociation threshold, the quantization function $F(E_b)$ reaches its universal low-κ_b limit, where it is solely determined by the inverse-cube tail potential. The threshold law (7) can then be related to the bound state energy E_b by inserting the right-hand side of Eq. (8),

$$-\frac{\tan\delta_0}{k} = \beta_3\ln(k\beta_3) + \frac{1}{\kappa_b} + O(k^1, \kappa_b^0), \tag{9}$$

where all constant terms have been omitted due to the occurrence of an additional unknown term $O(\kappa_b^0)$.

Higher angular momenta.—In an actual three-dimensional system, higher partial waves need to be taken into account, in order to obtain dependable results for the cross sections.

While in the limit of low energies the elastic cross section is—for potentials that fall off faster than $-1/r^3$—dominated by the s-wave contribution and assumes its threshold value $\sigma \sim 4\pi a^2$, the elastic cross section diverges at low energies in the presence of a $-1/r^3$ potential tail. In contrast to potentials that fall off faster, partial waves with nonzero angular momentum affect the cross section for elastic collisions by potentials with attractive inverse-cube tails even in the low-energy limit. The leading-order term of the phase shift in higher partial waves $l \geq 1$ is given by

$$\tan\delta_{l\geq 1} = \frac{1}{2l(l+1)}(k\beta_3) + O(k^2), \tag{10}$$

as can be obtained from the Born approximation [16]. It contains no information about the short-range part of the interaction potential.

The total cross section is given by the sum over all partial cross sections $\sigma_l = 4\pi(2l+1)\sin^2\delta_l/k^2$. In order to determine the low-energy behavior of the total cross section for elastic collisions to lowest order in the wave number k, all terms of order k need to be accounted for, especially in the expansion of $\tan\delta_0$ [see Eq. (7)]. The s-wave contribution $\sigma_{l=0}$ to the total cross section is given by

$$\sigma_{l=0} = 4\pi\beta_3^2\left[\ln(2k\beta_3) + \frac{\pi}{\tan(\pi\Delta)} + 3\gamma - \frac{3}{2}\right]^2 + O(k), \tag{11}$$

which is divergent in the limit of low collision energies.

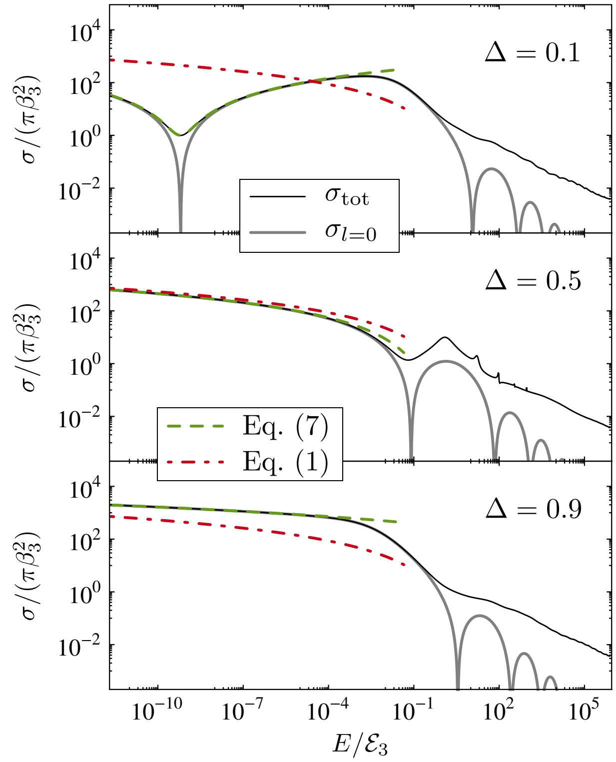

FIG. 2 (color online). Total cross sections for elastic scattering (solid black lines) are plotted against the collision energy for different values of the threshold quantum number's remainder $\Delta = \{0.1, 0.5, 0.9\}$. The corresponding s-wave contributions are shown as solid gray lines. The low-energy limit of the exact cross section is perfectly reproduced by the prediction via the correct threshold law (7), which is shown as the dashed line. The prediction via the simple form (1) (dotted line) is only a crude approximation to the exact cross section.

Since the contributions of partial waves with $l \geq 1$ to the low-energy limit of the total cross section are universal in the sense that they do not depend on the peculiarities of the potential at short distances [cf. Eq. (10)], they can be summed up in a straightforward way. This yields

$$\sigma_{\text{tot}} = \sigma_{l=0} + \sum_{l=1}^{\infty} \sigma_l = \sigma_{l=0} + \pi\beta_3^2 + O(k) \quad (12)$$

for the total cross section. The partial cross sections do not depend on the actual sign of $\tan\delta_l$; in the low-energy limit, the total contribution from partial waves with $l \geq 1$ is thus the same as for a repulsive $1/r^3$ potential (cf. Ref. [10]).

The three panels of Fig. 2 show total elastic cross sections in the presence of a $-C_3/r^3$ potential tail for different values of the threshold quantum number's remainder $\Delta = \{0.1, 0.5, 0.9\}$. In each panel, the solid black line gives the exact results for the total cross section σ_{tot} as obtained from numerically solving the Schrödinger equation (2); its s-wave contribution, corresponding to the results presented in Fig. 1, is shown as the gray line. In the case of $\Delta = 0.5$, shape resonances of considerable width are visible at $E \sim 10^2\mathcal{E}_3$. On the high-energy side of the range plotted in Fig. 2, the total elastic cross section is essentially given by the semiclassical estimate $\sigma_{\text{tot}} \sim 3\pi\beta_3^2\sqrt{\mathcal{E}_3/E}$ (see, e.g., Refs. [28,29]). The dashed lines show the results of Eq. (12) with the s-wave contribution from Eq. (11) for the respective value of the remainder Δ. They perfectly reproduce the exact results in the low-energy limit. Taking Eq. (12) with only the s-wave contribution as obtained with Eq. (1) yields the dot-dashed lines, which are only poor approximations to the respective exact cross sections. The upper panel shows a minimum in the cross section at around $E \sim 10^{-9}\mathcal{E}_3$, which is reminiscent of the Ramsauer-Townsend effect (see, e.g., Ref. [13]). However, the total cross section does not drop below $\pi\beta_3^2$, which is the threshold contribution of the partial waves with nonvanishing angular momentum [cf. Eq. (12)]. The exact results presented in Fig. 2 are universal for scattering by a potential with a $-1/r^3$ tail and the respective values of the threshold quantum number's remainder Δ.

Conclusions.—We have derived an explicit form of the threshold law (7) for attractive inverse-cube interactions, which is the main result of this Letter and is not given in the existing literature up to the present day. While a finite value of the scattering length does not exist in the presence of an inverse-cube tail potential, the threshold quantum number's remainder Δ offers a convenient parametrization of the asymptotic form of the regular solution (3) and introduces effects due to the short-range part of the potential into the threshold law (7). A further new result is the connection of the threshold law to the binding energy of a weakly bound state as established via Eq. (9).

While the results presented are obtained for elastic collisions involving only one channel, they can be extended to elastic scattering in the presence of channel coupling; Feshbach resonances are included according to the scheme presented in Ref. [30].

Despite the obvious theoretical interest in the knowledge of a threshold law for attractive inverse-cube interactions, the question remains whether it is or will be applicable in realistic situations. The system of aligned dipolar molecules confined to one dimension is a promising candidate for studying dipolar interactions at ultracold temperatures. The two-body interaction potentials for different configurations of this system have recently been calculated [31]. For typical values of the coefficient C_3, in a system of aligned KRb (LiNa) molecules, the accuracy of the threshold law (7) could be tested at temperatures in the nanokelvin (microkelvin) regime. This is indeed ultracold, but does not go beyond the scope of today's experiments. Theoretical studies of the corresponding many-body system, such as Ref. [32], could benefit from using Eq. (7) for the mediation of effective interactions at low collision energies.

The author is grateful to Harald Friedrich for helpful discussions and acknowledges support from the Deutsche Forschungsgemeinschaft (FR 591/17-1).

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