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Zero-energy bound or quasibound states and their implications for diatomic systems with an asymptotic van der Waals interaction

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Using an *l*-insensitive quantum defect theory, we derive a set of universal properties, both spectral and scattering, that are shared by diatomic systems with an asymptotic van der Waals interaction and having a zero-energy bound or a quasibound state of angular momentum l_b. The ^{133}Cs dimer is studied as an example. Systems that are close to having a bound or a quasibound state at the threshold are also discussed.

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For a quantum system with an asymptotic interaction of the form of $-C_n/r^n$ with $n>2$, it is possible to have a bound (in the case of $l>0$) or a quasibound state (in the case of $l=0$) right at the threshold that is characterized by a wave function with an asymptotic behavior of $u(r)\to A/r^l$ in the limit of large r. Recent developments in cold-atom physics have led to considerable interest in diatomic systems that have or are close to having such a state because of their special scattering characteristics [1]. Systems of this type are also of interest in the study of three-body dynamics, such as the existence of Efimov states [2], and in many-body physics, where they can be good candidates for going beyond the weak-coupling regime of the Bose-Einstein condensation (BEC) [3].

While the effective range expansion has provided insight into diatomic systems with a zero-energy quasibound *s* state [1], it is not useful for systems with zero-energy bound states of $l\neq 0$. The long-range character of the van der Waals interaction is such that the scattering length is not defined for $l>1$ and the effective range is not defined for $l>0$ [4,5]. Even for the *s* wave, the effective range expansion is not applicable beyond the k^2 term [5], implying that the energy range over which it is applicable is very limited.

Based on an *l*-insensitive quantum-defect theory [6], we present in this Rapid Communication a general discussion of the properties of diatomic systems with an asymptotic van der Waals interaction and having a zero-energy bound or quasibound state of angular momentum l_b. We show that such states do not appear in isolation. They appear in sets. Specifically, if there is a bound or quasibound state of angular momentum l_b right at or very close to the threshold, there are also bound or quasibound states of angular momenta $l=l_b\pm 4j$ ($l\geqslant 0$ and $j=1,2,\dots$) that are right at or very close to the threshold. For example, if a system is close to having a quasibound *s* state at the threshold, it will also be close to having a bound *g* state at the threshold. As a related conclusion, diatomic systems with an asymptotic van der Waals interaction and having zero-energy bound or quasibound states can be classified into four types, each with its characteristic spectral and scattering properties, which will be presented and discussed.

The key concept of the *l*-insensitive quantum-defect theory [6] is the following. Under proper conditions that are satisfied by most diatomic systems [6], the bound spectra and scattering of *different* relative angular momenta can be described by the *same* short-range parameter K^c, in combination with solutions for the long-range interactions [7,8]. To briefly summarize, the bound spectra are given by crossing points between a set of universal functions $\chi_l^c(\epsilon_s)$, which come from the solutions for the asymptotic potential, and a short-range parameter K^c, which is, to a good approximation, independent of both the energy and the angular momentum in the threshold region (see Fig. 1). The χ_l^c functions for the van der Waals interaction, $-C_6/r^6$, are given explicitly in [6]. They are functions of a scaled energy ϵ_s defined by

$$\epsilon_s=\frac{1}{16}\frac{\epsilon}{(\hbar^2/2\mu)(1/\beta_6)^2}, \tag{1}$$

where $\beta_6\equiv(2\mu C_6/\hbar^2)^{1/4}$.

Above the threshold, the scattering K matrix is given by the same parameter K^c through the equation

$$K_l\equiv\tan\delta_l=(K^cZ_{gg}^c-Z_{fg}^c)(Z_{ff}^c-K^cZ_{gf}^c)^{-1}, \tag{2}$$

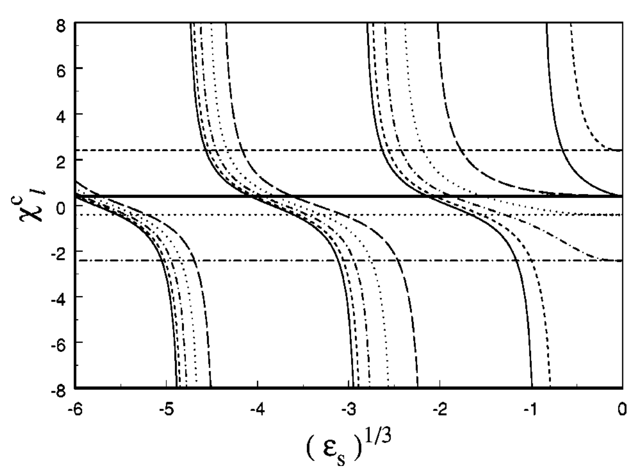

FIG. 1. The dimensionless χ_l^c functions for the $-C_6/r^6$ interaction plotted vs $(\epsilon_s)^{1/3}$. Solid line, $l=0$; dashed line, $l=1$; dash-dotted line, $l=2$; dotted line, $l=3$; long dashed line, $l=4$. For systems satisfying $\beta_6\gg r_0$, the bound spectra in the threshold region are given by the crossing points of χ_l^c functions with a single horizontal line representing $K^c=$const. The four horizontal lines in the figure represent four classes of diatomic systems that have zero-energy bound or quasibound states.

TABLE I. Scaled bound-state energies ϵ_s, of a quantum system with an asymptotic van der Waals interaction and a set of zero-energy bound or quasibound states of $l_b=4j$, $j=0,1,2,\ldots$. The symmetry of the system may be such that only the even or only the odd partial wave states are allowed.

$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	$l=5$
0.0					
−9.879	−8.789	−6.668	−3.648	0.0	
−68.12	−66.03	−61.89	−55.74	−47.69	−37.87
−217.7	−214.6	−208.5	−199.3	−187.2	−172.2

where the Z^c matrix comes again from the solutions for the van der Waals potential [7] and is given explicitly by

$$Z^c_{ff}=\frac{2^{-1/2}G_{\epsilon l}(\nu)\cos\pi(\nu-\nu_0)}{(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin\pi\nu}\times\{[1-(-1)^l M_{\epsilon l}\tan\pi(\nu-\nu_0)]\sin(\pi\nu/2)X_{\epsilon l}+[1+(-1)^l M_{\epsilon l}\tan\pi(\nu-\nu_0)]\cos(\pi\nu/2)Y_{\epsilon l}\},\tag{3}$$

$$Z^c_{fg}=\frac{2^{-1/2}G_{\epsilon l}(\nu)\cos\pi(\nu-\nu_0)}{(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin\pi\nu}\times\{[\tan\pi(\nu-\nu_0)-(-1)^l M_{\epsilon l}]\sin(\pi\nu/2)X_{\epsilon l}+[\tan\pi(\nu-\nu_0)+(-1)^l M_{\epsilon l}]\cos(\pi\nu/2)Y_{\epsilon l}\},\tag{4}$$

$$Z^c_{gf}=\frac{2^{-1/2}G_{\epsilon l}(\nu)\cos\pi(\nu-\nu_0)}{(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin\pi\nu}\times\{[1+(-1)^l M_{\epsilon l}\tan\pi(\nu-\nu_0)]\cos(\pi\nu/2)X_{\epsilon l}-[1-(-1)^l M_{\epsilon l}\tan\pi(\nu-\nu_0)]\sin(\pi\nu/2)Y_{\epsilon l}\},\tag{5}$$

$$Z^c_{gg}=\frac{2^{-1/2}G_{\epsilon l}(\nu)\cos\pi(\nu-\nu_0)}{(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin\pi\nu}\times\{[\tan\pi(\nu-\nu_0)+(-1)^l M_{\epsilon l}]\cos(\pi\nu/2)X_{\epsilon l}-[\tan\pi(\nu-\nu_0)-(-1)^l M_{\epsilon l}]\sin(\pi\nu/2)Y_{\epsilon l}\}.\tag{6}$$

TABLE II. Same as Table I, except for $l_b=4j+1$.

$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	$l=5$
−0.2828	0.0				
−18.23	−16.89	−14.25	−10.42	−5.568	0.0
−95.27	−92.94	−88.29	−81.39	−72.31	−61.17
−274.4	−271.1	−264.4	−254.5	−241.4	−225.1

TABLE III. Same as Table I, except for $l_b=4j+2$.

$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	$l=5$
−1.577	−1.001	0.0			
−30.27	−28.68	−25.54	−20.92	−14.97	−7.885
−128.8	−126.2	−121.1	−113.4	−103.3	−90.89
−340.1	−336.6	−329.4	−318.8	−304.7	−287.1

Here $M_{\epsilon l}=G_{\epsilon l}(-\nu)/G_{\epsilon l}(\nu)$, with ν, $X_{\epsilon l}$, $Y_{\epsilon l}$, and $G_{\epsilon l}$ being defined in [7]. They are all functions of the scaled energy ϵ_s. The Z^c matrix is related to the Z matrix defined in [7] by a linear transformation.

Near the threshold, the χ^c_l function [6] exhibits the behavior

$$\chi^c_l \xrightarrow{\epsilon_s\to 0} \tan(\pi\nu_0/2)=\tan(l\pi/4+\pi/8).\tag{7}$$

A diatomic system with a bound or quasibound state of angular momentum l_b right at the threshold must therefore have a short-range parameter K^c given by

$$K^c=\tan(l_b\pi/4+\pi/8).\tag{8}$$

Depending on the value of l_b, there are four possible values that K^c can take. Since states of different angular momenta are all described by the same K^c, and since χ^c_l has the same zero-energy limit for l and $l\pm 4j$, it is easily deduced that zero-energy bound or quasibound states come in sets and can be classified into four types according to

$$K^c=\begin{cases}+\tan(\pi/8), & l_b=4j\\ +\tan(3\pi/8), & l_b=4j+1\\ -\tan(3\pi/8), & l_b=4j+2\\ -\tan(\pi/8), & l_b=4j+3,\end{cases}\tag{9}$$

where $j=0,1,2,\ldots$. For the type of system characterized by $K^c=\tan(\pi/8)$, K^c crosses a set of χ^c_l with $l=4j$ right at the threshold, leading to a set of zero-energy bound or quasibound states of $l_b=4j$. Similarly, three other values of K^c describe three other types of systems with sets of zero-energy bound states of $l_b=4j+1$, $l_b=4j+2$, and $l_b=4j+3$, respectively. Each type of system has a unique set of bound spectra and scattering properties, as specified in Tables I–IV and Figs. 2–5. The bound spectra are determined as in Fig. 1. The scattering properties are determined from Eq. (2). From this classification, it is also clear that if a system is close to having a zero-energy bound or quasibound

TABLE IV. Same as Table I, except for $l_b=4j+3$.

$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	$l=5$
−4.553	−3.716	−2.124	0.0		
−46.68	−44.84	−41.19	−35.81	−28.80	−20.32
−169.4	−166.6	−160.9	−152.5	−141.4	−127.7
−415.6	−411.8	−404.2	−392.8	−377.7	−358.9

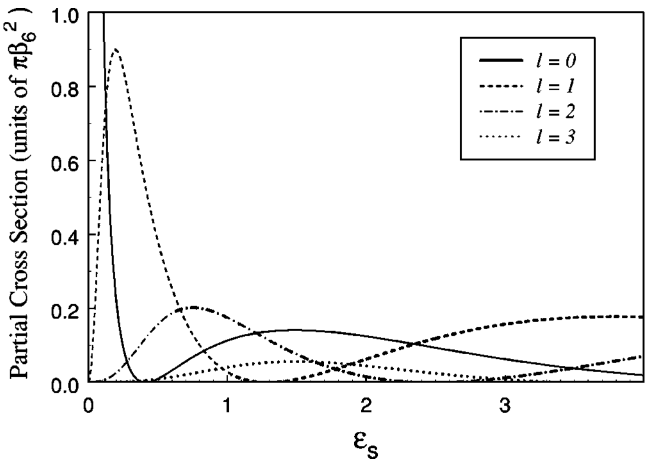

FIG. 2. Partial scattering cross sections for a quantum system with an asymptotic van der Waals interaction and a set of zero-energy bound or quasibound states of $l_b=4j$, $j=0,1,2,\ldots$. The cross sections should be multiplied by 2 if the symmetry is such that only the even or only the odd partial waves are allowed.

state of angular momentum l_b [namely, having a K^c that is close to one of the four values in Eq. (9)], it will also be close to having zero-energy bound or quasibound states of angular momenta $l=l_b\pm 4j$, since the zero-energy limits of χ_l^c are the same for l_b and $l_b\pm 4j$. Depending on whether K^c is slightly greater than or smaller than one of the four values in Eq. (9), those states show up either as a set of bound states with $\epsilon_s \ll 1$ or as narrow shape resonances, for $l>0$, and an increase in the density of states, for $l=0$, right above the threshold.

Table I and Fig. 2 give, respectively, the bound spectra and the partial cross sections for the class of systems having bound or quasibound states of $l_b=4j=0,4,8,\ldots$, right at the threshold. They are characterized by $K^c=\tan(\pi/8)$. While Eq. (2) and Fig. 2 are applicable over a wide range of energies and include much more than just the threshold behaviors, it is still of interest to look more closely at whether and how the threshold behaviors may be effected by the presence of the zero-energy bound or quasibound states. From

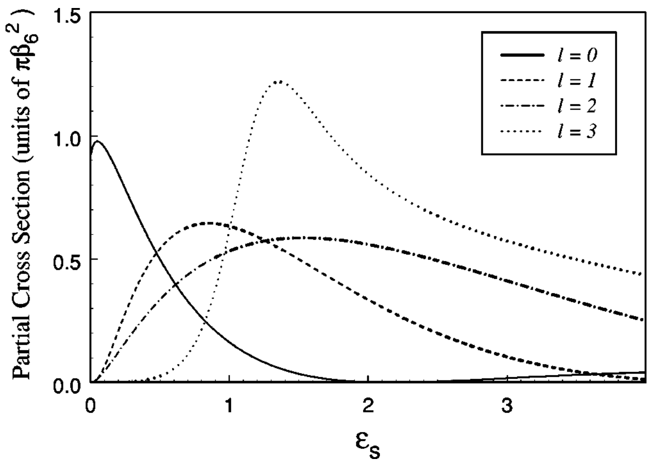

FIG. 4. Same as Fig. 2, except for $l_b=4j+2$.

the K^c parameter, the s-wave scattering length can generally be found through the relationship [9]

$$a_{l=0}=\frac{2^{3/2}\pi}{[\Gamma(1/4)]^2}\frac{K^c+\tan(\pi/8)}{K^c-\tan(\pi/8)}\beta_6, \qquad (10)$$

and the corresponding s-wave effective range can be found through the relationship in [5]. For the class of systems characterized by $K^c=\tan(\pi/8)$, the s-wave scattering length is $a_{l=0}=\infty$, as expected, and the s-wave effective range is $r_{el=0}=(3\pi)^{-1}[\Gamma(1/4)]^2\beta_6$. The s-wave partial cross section diverges at the threshold according to [9]

$$\sigma_{l=0}\xrightarrow{\epsilon\to 0}(4\pi/k^2)[1+(1/4)r_{el=0}^2k^2]^{-1}, \qquad (11)$$

which, other than the specific value for $r_{el=0}$, could have been predicted by the effective range expansion. The threshold behaviors for the higher partial waves [5] are not in this case effected by the presence of the zero-energy bound and quasibound states of $l_b=4j=0,4,8,\ldots$.

Table II and Fig. 3 give, respectively, the bound spectra and the partial cross sections for the class of systems that are characterized by $K^c=\tan(3\pi/8)$ and have zero-energy

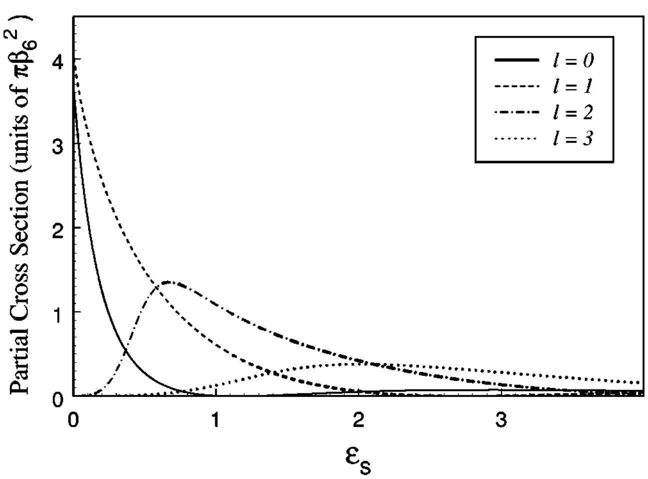

FIG. 3. Same as Fig. 2, except for $l_b=4j+1$.

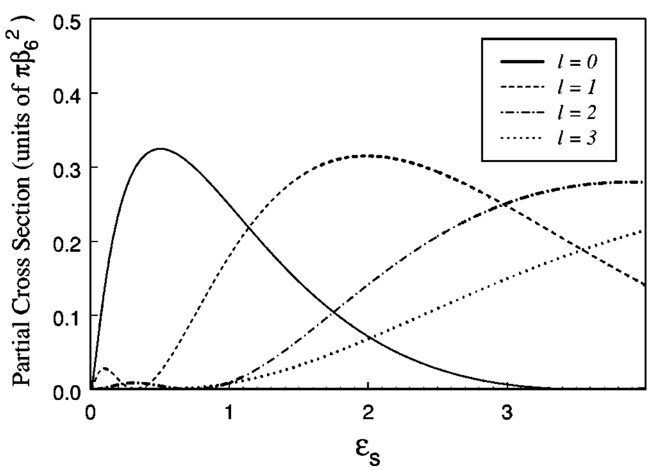

FIG. 5. Same as Fig. 2, except for $l_b=4j+3$.

bound states of $l_b=4j+1=1,5,9,\ldots$. In this case, the *p*-wave partial cross section goes to a constant instead of zero at the threshold, according to [9]

$$\sigma_{l=1}/(\pi\beta_6^2) \xrightarrow{\epsilon\to 0} 3^{-3}[\Gamma(3/4)]^{-4}5^2\pi^2. \tag{12}$$

Systems of this type should be of interest in the study of a cold atomic Fermi gas [10], as evaporative cooling remains effective towards zero temperature. The threshold behaviors for the lower and the higher partial waves are not effected by the presence of the zero-energy bound states. In particular, the *s*-wave scattering length is given in this case by $a_{l=0}=4\pi[\Gamma(1/4)]^{-2}\beta_6$, and the effective range is given by $r_{el=0}=(6\pi)^{-1}[\Gamma(1/4)]^2\beta_6$.

Table III and Fig. 4 give, respectively, the bound spectra and the partial cross sections for the class of systems that are characterized by $K^c=-\tan(3\pi/8)$ and have bound states of $l_b=4j+2=2,6,10,\ldots$, right at the threshold. The threshold behaviors [5] for this class of systems are not effected by the presence of the zero-energy bound states. The *s*-wave scattering length is given by $a_{l=0}=2\pi[\Gamma(1/4)]^{-2}\beta_6$, and the effective range is given by $r_{el=0}=(3\pi)^{-1}[\Gamma(1/4)]^2\beta_6$.

Table IV and Fig. 5 give, respectively, the bound spectra and the partial cross sections for the class of systems that are characterized by $K^c=-\tan(\pi/8)$ and have bound states of $l_b=4j+3=3,7,\ldots$, right at the threshold. In this case, the *s*-wave scattering length goes to zero and the effective range goes to infinity. The *s*-wave threshold behavior cannot be described by the effective range expansion. It is given instead by [9]

$$\sigma_{l=0}/(\pi\beta_6^2) \xrightarrow{\epsilon\to 0} 3^{-2}[\Gamma(1/4)]^{-4}2^6\pi^2(k\beta_6)^4, \tag{13}$$

which goes to zero as k^4. The threshold behaviors [5] for the higher partial waves are not effected by the presence of the zero-energy bound states.

The characteristic spectra presented in Tables I–IV and the partial cross sections presented in Figs. 2–5 are all given in reduced units. The energies are scaled according to Eq. (1) and the cross sections are scaled by $\pi\beta_6^2$. They are, however, easily converted into absolute scales by using the parameters μ and C_6 for a particular system. As an example, we present in Table V predictions of the bound spectra of the ^{133}Cs dimer in states characterized by quantum number $F_1=F_2=4$, $F=8$, $l=0,2,4,6$, and $T=F+l$ [11], assuming that it has a triplet quasibound *s* state right at the threshold [1]. They are obtained using $\mu=121\,135.89$ a.u. and $C_6=6851$ a.u. [12]. The partial cross sections in Fig. 2 can be converted into absolute scales for cesium in a similar fashion.

TABLE V. Bound-state energies (in GHz) of $^{133}Cs_2$ with quantum numbers $F_1=4$, $F_2=4$, $F=8$, $l=0,2,4,6$, and $T=F+l$, assuming that it has a zero-energy quasibound triplet *s* state.

$l=0$	$l=2$	$l=4$	$l=6$
0.0			
−0.1054	−0.07112	0.0	
−0.7266	−0.6601	−0.5087	−0.2821
−2.322	−2.224	−1.997	−1.647
−5.349	−5.219	−4.918	−4.450
−10.27	−10.11	−9.730	−9.144

In conclusion, we have presented a general discussion of the properties of quantum systems with an asymptotic van der Waals interaction and having zero-energy bound or quasibound states. The classification of these systems into four types, and the four sets of universal properties associated with them, are not only interesting by themselves. They also provide the reference points for an understanding of any diatomic system with an asymptotic van der Waals interaction. In the example of the ^{133}Cs dimer, for instance, if the bound-state energies are found experimentally [13] to be slightly higher than those presented in Table V, it could mean that the K^c parameter is slightly smaller than $\tan(\pi/8)$ [14]. The scattering length would in this case be large (compared to β_6) and negative, and the system should show a narrow *g*-wave shape resonance right above the threshold. On the other hand, if the bound-state energies are found [13] to be slightly lower than those presented in Table V, it could mean that the K^c parameter is slightly greater than $\tan(\pi/8)$ [14]. The scattering length would in this case be large and positive, and the system should not show a *g*-wave shape resonance right above the threshold.

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