Highly excited bound-state resonances of short-range inverse power-law potentials

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Abstract We study analytically the radial Schrödinger equation with long-range attractive potentials whose asymptotic behaviors are dominated by inverse power-law tails of the form $V(r) = -\beta_n r^{-n}$ with $n > 2$. In particular, assuming that the effective radial potential is characterized by a short-range infinitely repulsive core of radius $R$, we derive a compact analytical formula for the threshold energy $E_{\text{max}}^{l} = E_{\text{max}}^{l}(n, \beta_n, R)$, which characterizes the most weakly bound-state resonance (the most excited energy level) of the quantum system.

1 Introduction

The Schrödinger differential equation with inverse power-law attractive potentials has attracted the attention of physicists and mathematicians since the early days of quantum mechanics. In particular, long-range power-law potentials play a key role in theoretical models describing the physical interactions of atoms and molecules (see [1–10] and the references therein).

It is well known that the attractive Coulombic potential is characterized by an infinite spectrum $\{E_k\}_{k=0}^{\infty}$ of stationary bound-state resonances with the asymptotic property $E_k \to 0^-$ as $k \to \infty$ [10]. On the other hand, attractive radial potentials whose asymptotic spatial behaviors are dominated by inverse power-law decaying tails of the form

$$V(r) = -\frac{\beta_n}{r^n} \quad \text{with} \quad n > 2$$

(1)

can only support a finite number of bound-state resonances [10]. In particular, it is interesting to note that, for generic values of the physical parameters $n$ and $\beta_n$, the discrete energy spectrum of an attractive inverse power-law potential of the form (1) terminates at some finite non-zero energy $E_{\max}(n, \beta_n)$ [1–11].

The main goal of the present paper is to present a simple and elegant mathematical technique for the calculation of the most excited energy levels $E_{\max}(n, \beta_n)$, which characterize the family (1) of attractive inverse power-law potentials. In particular, below we shall derive a compact analytical formula for the threshold (maximal) energies $E_{\max}(n, \beta_n)$ which characterize the most weakly bound-state resonances (the most excited energy levels) of the radial Schrödinger equation with the inverse power-law attractive potentials (1).

2 Description of the system

We shall analyze the physical properties of a quantum system whose stationary resonances are determined by the radial Schrödinger equation

$$\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r) \right] \psi_l = E \psi_l ,$$

(2)

where the effective radial potential $V(r)$ in (2) is characterized by a long-range inverse power-law attractive part and a short-range infinitely repulsive core. Specifically, we shall consider a composed radial potential of the form

1 Note that the most excited energy levels $E_{\max}(n, \beta_n)$ correspond to the most weakly bound-state resonances of the inverse power-law binding potentials (1).
2 It is worth mentioning that the weakly bound-state resonances which characterize the inverse power-law potentials (1) play a key role in the physical description of the scattering of low-energy atoms and molecules and in widely used theoretical models of the Bose–Einstein condensation phenomenon [9].
3 Here $\mu$ is the effective (reduced) mass of the physical system and $l$ is the spherical harmonic index of the quantum mode.
\[ V(r) = \begin{cases} +\infty & \text{for } r \leq R \\ -\frac{\mu}{2r^2} & \text{for } r > R \end{cases} \] (3)

The bound-state \((E < 0)\) resonances of the Schrödinger differential equation (2) that we shall analyze in the present paper are characterized by exponentially decaying radial eigenfunctions at spatial infinity:

\[ \psi_l(r \rightarrow \infty) \sim e^{-\kappa r}, \] (4)

where

\[ \kappa^2 \equiv -\frac{2\mu}{\hbar^2}E \text{ with } \kappa \in \mathbb{R}. \] (5)

In addition, the repulsive core of the effective radial potential (3) dictates the inner boundary condition

\[ \psi_l(r = R) = 0 \] (6)

for the characteristic radial eigenfunctions.

The Schrödinger equation (2), supplemented by the radial boundary conditions (4) and (6), determine the discrete spectrum of bound-state eigen-wavenumbers \(\{\kappa(n, \beta_n, R)\}\) (or equivalently, the discrete spectrum of binding energies \(E(n, \beta_n, R)\)) which characterize the effective radial potential (3). As we shall explicitly show in the next section, the most weakly bound-state resonance (that is, the most excited energy level), which characterizes the quantum system (3), can be determined analytically in the regime [12]

\[ \kappa r_n \ll 1 \] (7)

of small binding energies, where the characteristic length scale \(r_n\) is defined by the relation

\[ r_n = \left( \frac{2\mu\beta_n}{(n-2)\hbar^2} \right)^{1/(n-2)}. \] (8)

\[ ^4 \text{We shall assume, without loss of generality, that } \kappa > 0. \]

\[ ^5 \text{Note that the strong inequality (7) corresponds to small resonant energies in the regime } (2\mu\beta_n^2/\hbar^2)^{p/(n-2)}E \ll 1 \text{ (see Eqs. (5) and (8)).} \]

\[ ^6 \text{It is important to point out that the special case of s-waves } (l = 0) \text{ has been studied in the highly important work of Gribakin and Flambaum [12], where it was explicitly proved that the energy of the most excited energy level can be expressed in the simple form } \kappa = 1/(\alpha - \bar{a}), \text{ where } \alpha \text{ and } \bar{a} \text{ are, respectively, the s-wave scattering length and the so-called average scattering length (see, in particular, Eqs. (3) and (29) of [12]). It is worth emphasizing, however, that the interesting work presented in [12] is based on the semi-classical WKB analysis, whereas in the present paper we shall present a full quantum-mechanical treatment of the physical system. In addition, in the present paper we shall extend the interesting results of [12] to the more generic physical regime of non-spherically symmetric higher partial wave functions (that is, our analytical results, to be derived below, are valid for generic values of the dimensionless physical parameter } l. \]

3 The resonance equation and its regime of validity

In the present section we shall analyze the radial Schrödinger equation

\[ \begin{cases} \frac{d^2}{dr^2} - \frac{1}{r^2} \left[ (kr)^2 + l(l+1) - (n-2)^2 \left( \frac{r_n}{r} \right)^{n-2} \right] \\ \psi_l(r; \kappa, r_n, n) = 0, \end{cases} \] (9)

which determines the spatial behavior of the bound-state eigenfunctions \(\psi_l(r)\) in the regime \(r > R\). As we shall explicitly show below, the characteristic radial equation (9) can be solved analytically in the two asymptotic radial regions \(r \ll 1/\kappa\) and \(r \gg r_n\). We shall then show that, for small resonant energies in the regime \(\kappa r_n \ll 1\) [see (7) (see footnote 5)], one can use a functional matching procedure in the overlapping region \(r_n \ll r \ll 1/\kappa\) in order to determine the binding energies \((E(n, r_n, R, l))\) (or equivalently, the eigen-wavenumbers \(\{\kappa(n, r_n, R, l)\}\)) which characterize the marginally bound-state resonances of the radial Schrödinger equation (2) with the effective binding potential (3).

We shall first solve the Schrödinger equation (9) in the radial region

\[ r \ll 1/\kappa, \] (10)

in which case one may approximate (9) by

\[ \left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{(n-2)^2 r_n^{n-2}}{r^n} \right] \psi_l = 0. \] (11)

The general solution of the radial differential equation (11) can be expressed in terms of the Bessel functions of the first and second kinds (see Eq. 9.1.53 of [13]):

\[ \psi_l(r) = A_1 r^{1/2} J_{\frac{2l+1}{n-2}} \left( \frac{r_n}{r} \right)^{(n-2)/2} + A_2 r^{1/2} Y_{\frac{2l+1}{n-2}} \left( \frac{r_n}{r} \right)^{(n-2)/2}, \] (12)

where \(\{A_1, A_2\}\) are normalization constants to be determined below. Using the small-argument \((r_n/r \ll 1)\) asymptotic behaviors of the Bessel functions (see Eqs. 9.1.7 and 9.1.9 of [13]), one finds from (12) the expression

\[ \psi_l(r) = A_1 \left( \frac{r_n^{1/2}}{r} \right)^{l/2} J_{\frac{2l+1}{n-2}} \left( \frac{r_n}{r} \right)^l - A_2 \left( \frac{r_n^{1/2}}{r} \right)^{l/2} \Gamma_{\frac{2l+1}{n-2}}(\frac{r}{r_n})^{l+1}, \] (13)

for the radial eigenfunction which characterizes the weakly bound (highly excited) states of the Schrödinger differential equation (9) in the intermediate radial region.
We shall next solve the Schrödinger equation (9) in the radial region
\[ r \gg r_n , \]
in which case one may approximate (9) by
\[ \left[ \frac{d^2}{dr^2} - \kappa^2 - \frac{l(l+1)}{r^2} \right] \psi_l = 0 . \] (16)

The general solution of the radial differential equation (16) can be expressed in terms of the Bessel functions of the first and second kinds (see Eq. 9.1.49 of [13]):
\[ \psi_l(r) = B_1 r^{\frac{l}{2}} J_{\frac{l+1}{2}}(i \kappa r) + B_2 r^{-\frac{l}{2}} Y_{\frac{l+1}{2}}(i \kappa r) , \] (17)
where \( \{B_1, B_2\} \) are normalization constants. Using the small-argument (\( \kappa r \ll 1 \)) asymptotic behaviors of the modified Bessel functions (see Eqs. 9.1.7 and 9.1.9 of [13]), one finds from (17) the expression
\[ \psi_l(r) = B_1 \frac{(i \kappa/2)^l}{l!} r^{l+1} - B_2 \frac{\Gamma\left(l + \frac{1}{2}\right)}{\pi (i \kappa/2)^{l+\frac{3}{2}}} r^{-l} \] (18)
for the radial eigenfunction which characterizes the weakly bound-state resonances (the highly excited states) of the Schrödinger differential equation (9) in the intermediate radial region
\[ r_n \ll r \ll 1/\kappa . \] (19)

Interestingly, for weakly bound-state resonances (that is, for small resonant wavenumbers in the regime \( \kappa r_n \ll 1 \)), the two expressions (13) and (18) for the characteristic eigenfunction \( \psi_l(r) \) of the radial Schrödinger equation (9) are both valid in the intermediate radial region \( r_n \ll r \ll 1/\kappa \) [see Eqs. (14) and (19)]. Note, in particular, that these two analytical expressions for the radial eigenfunction \( \psi_l(r) \) are characterized by the same functional (radial) behavior. One can therefore express the coefficients \( \{B_1, B_2\} \) of the radial solution (17) in terms of the coefficients \( \{A_1, A_2\} \) of the radial solution (12) by matching the two mathematical expressions (13) and (18) for the characteristic radial eigenfunction \( \psi_l(r) \).

\(^7\) As we shall explicitly show below, the normalization constants \( \{B_1, B_2\} \) of the radial solution (17) can be determined by a functional matching procedure.

in the intermediate radial region \( r_n \ll r \ll 1/\kappa . \) This functional matching procedure yields the relations
\[ B_1 = -A_2 \frac{(l + \frac{1}{2}) \Gamma\left(l + \frac{1}{2}\right) \Gamma\left(\frac{2l+1}{n-2}\right)}{\pi \Gamma\left(\frac{2l+1}{n-2}\right)} \] (20)
and
\[ B_2 = -A_1 \frac{(l + \frac{1}{2}) \Gamma\left(l + \frac{1}{2}\right) \Gamma\left(\frac{2l+1}{n-2}\right)}{(i \kappa r_n)^{l+\frac{1}{2}}} . \] (21)

We are now in a position to derive the resonance equation which determines the binding energies \( \{E(n, r_n, l)\} \) [or equivalently, the eigen-wavenumbers \( \{\kappa(n, r_n, l)\} \) of the weakly bound (highly excited) states which characterize the radial Schrödinger equation (2) with the effective radial potential (3). Using Eqs. 9.2.1 and 9.2.2 of [13], one finds the asymptotic spatial behavior
\[ \psi_l(r \to \infty) = B_1 \sqrt{2/\pi \kappa} \cdot \cos(i \kappa r - l \pi/2 - \pi/2) + B_2 \sqrt{2/\pi \kappa} \cdot \sin(i \kappa r - l \pi/2 - \pi/2) \] (22)
for the radial eigenfunction (17). Taking account of the boundary condition (4), which characterizes the bound-state resonances of the radial Schrödinger equation (2), one deduces from (22) the simple relation
\[ B_2 = i B_1 . \] (23)

Substituting Eqs. (20) and (21) into (23), one obtains the characteristic resonance equation
\[ \left(\frac{i \kappa r_n}{2}\right)^{2l+1} = i \frac{2}{n-2} \left[ \frac{(l + \frac{1}{2}) \Gamma\left(l + \frac{1}{2}\right) \Gamma\left(\frac{2l+1}{n-2}\right)}{\pi \Gamma\left(\frac{2l+1}{n-2}\right)} \right]^2 \frac{A_2}{A_1} \] (24)
for the highly excited bound-state resonances which characterize the Schrödinger equation (2) with the effective radial potential (3).

\(^8\) Note that the coefficients \( \{A_1, A_2\} \) and \( \{B_1, B_2\} \) of the radial solutions (12) and (17) satisfy the compact relation \( B_1 B_2/A_1 A_2 = (n-2)/2 \).

\(^9\) We recall that \( 0 < \kappa \in \mathbb{R} \) [see Eq. (5) and (see footnote 4)]. Thus, from Eq. (22) one finds \( \psi_l(r \to \infty) \sim e^{-\kappa r} \to 0 \) for \( B_2 = i B_1 \).
4 The resonant binding energy of the most excited energy level

The dimensionless ratio \( A_2 / A_1 \), which appears in the resonance equation (24) can be determined by the inner boundary condition (6) which is dictated by the short-range repulsive part of the effective radial potential (3). In particular, substituting (12) into (6), one finds

\[
A_2 = - \frac{J_{2l+1}^{(n+1)}}{\frac{2}{R_{n+1}}} \left[ 2 \left( \frac{r}{R} \right)^{(n-2)/2} \right] \]

Substituting the dimensionless ratio (25) into the resonance equation (24), one finally finds the expression\(^{10}\)

\[
\kappa r_n = \left\{ \begin{aligned}
&\frac{(-1)^{l+1}}{n-2} \left[ \frac{2^{2l+1} (l+1)}{\pi} \Gamma \left( \frac{l+\frac{1}{2}}{2} \right) \Gamma \left( \frac{2l+1}{n-2} \right) \right]^2 \\
&\frac{J_{2l+1}^{(n+1)}}{\frac{2}{R_{n+1}}} \left[ 2 \left( \frac{r}{R} \right)^{(n-2)/2} \right]^{1/(2l+1)} \\
&Y_{2l+1}^{(n+1)} \left[ 2 \left( \frac{r}{R} \right)^{(n-2)/2} \right]^{1/(2l+1)}
\end{aligned} \right\}
\]

(26)

for the dimensionless resonant wavenumber which characterizes the most excited energy level (the most weakly bound-state resonance) of the radial Schrödinger equation (2) with the effective binding potential (3).

It is worth emphasizing again that the analytically derived resonance equation (24) is valid in the regime [see (14) and (19)]\(^{11}\)

\[
\kappa r_n \ll 1
\]

(27)

\(\kappa\) of small binding energies. Taking account of Eq. (26), one realizes that the small wavenumber requirement (27) is satisfied for

\[
2 \left( \frac{r}{R} \right)^{(n-2)/2} \simeq j_{\frac{2l+1}{n-2}, k} \equiv 2 \left( \frac{r}{R} \right)^{(n-2)/2} - j_{\frac{2l+1}{n-2}, k} \ll 1,
\]

(28)

where \( j_{\ell, k} \equiv \mathcal{J}_\ell(x) \) are the positive zeros of the Bessel function \( J_\ell(x) \). Defining the dimensionless small quantity

\[
\Delta_k \equiv 2 \left( \frac{r}{R} \right)^{(n-2)/2} - j_{\frac{2l+1}{n-2}, k} \ll 1,
\]

(29)

one finds from (26) the expression\(^{12,13}\)

\[
\kappa r_n = \left\{ \begin{aligned}
&\frac{(-1)^l}{\pi(n-2)} \left[ (2l+1)! \Gamma \left( \frac{2l+1}{n-2} \right) \right]^2 \\
&\frac{J_{\frac{2l+1}{n-2}, k}}{Y_{\frac{2l+1}{n-2}, k} \Delta_k} \left[ \frac{2}{n-2} \right]^{(n-2)/2} \end{aligned} \right\}
\]

(30)

for the smallest resonant wavenumber which characterizes the effective binding potential (3).

5 Summary

We have studied analytically the Schrödinger differential equation with attractive radial potentials whose asymptotic behaviors are dominated by inverse power-law tails of the form \( V(r) = -\beta_n r^{-\nu} \) with \( n > 2 \). These long-range radial potentials are of great importance in physics and chemistry. In particular, they provide a quantitative description for the physical interactions of atoms and molecules [1–10].

Using a low-energy matching procedure, we have derived the analytical expression [see Eqs. (5), (8), (29), and (30)]

\[12\text{ Here we have used the Taylor expansions}\]

\[\frac{J_{\frac{2l+1}{n-2}, k}}{Y_{\frac{2l+1}{n-2}, k} \Delta_k} \cdot \Delta_k + O(\Delta_k^2) = -j_{\frac{2l+1}{n-2}, k} \cdot \Delta_k + O(\Delta_k^2) \text{ [see Eq. 9.1.27d of [13]]} \]

\[Y_{\frac{2l+1}{n-2}, k} \left[ \frac{2}{n-2} \right]^{(n-2)/2} = \frac{2}{n-2} \left[ \frac{2}{n-2} \right]^{(n-2)/2} + j_{\frac{2l+1}{n-2}, k} + \Delta_k \]

\[\frac{Y_{\frac{2l+1}{n-2}, k} \left( j_{\frac{2l+1}{n-2}, k} + \Delta_k \right)}{Y_{\frac{2l+1}{n-2}, k} \left( j_{\frac{2l+1}{n-2}, k} \right)} = \frac{Y_{\frac{2l+1}{n-2}, k} \left( j_{\frac{2l+1}{n-2}, k} + \Delta_k \right)}{Y_{\frac{2l+1}{n-2}, k} \left( j_{\frac{2l+1}{n-2}, k} \right)} + O(\Delta_k) \text{. In addition, we have used here Eq. 6.1.12 of [13]} \]

\[\text{13 It can be checked directly that the dimensionless ratio}\]

\[j_{\frac{2l+1}{n-2}, k} / j_{\frac{2l+1}{n-2}, k} \text{ in (30) is a positive definite expression. Thus, the assumption } \kappa > 0 \text{ (see footnote 4) corresponds to the relation } (-1)^l \cdot \Delta_k > 0.\]
with \[12\].

\[
\left(\frac{2\mu\beta_n}{\hbar^2}\right)^{\frac{n}{n^2}} \cdot E_{\text{max}}^{\text{max}}(n, l)
\]

\[
= - \left\{ \frac{(-1)^l}{\pi(n - 2)} \left(2l + 1\right)! \left(n - 2\right)^{\frac{2l+1}{2}} \Gamma\left(\frac{2l + 1}{n - 2}\right) \right\}^2
\]

\[
\frac{\left(2\mu\beta_n\right)^{\frac{n}{n^2}}}{\hbar^2} \cdot E_{\text{max}}^{\text{max}}(n \gg 1, l)
\]

\[
= - \left\{ \frac{(-1)^l}{\pi} \left[2l + 1\right]! \left(n - 2\right)^{\frac{2l+1}{2}} \Gamma\left(\frac{2l + 1}{n - 2}\right) \right\}^2 \frac{J_l(j_{0,k})}{Y_0(j_{0,k})} \Delta_k
\]

\[
Y_{2l+1}(\frac{j_{2l+1}}{\pi}, k)
\]

\[
\frac{2\mu\beta_r}{\hbar^2} \cdot E_{\text{max}}^{\text{max}}(n \gg 1, l) = - \left[ \frac{\pi}{\pi} \cdot \frac{\left(2\mu\beta_r\right)^{\frac{n}{n^2}}}{\hbar^2} \right]^{\frac{n}{n^2}} \cdot E_{\text{max}}^{\text{max}}(n \gg 1, l)
\]

for the characteristic threshold energy which characterizes the most excited energy level (the most weakly bound-state resonance) of the radial Schrödinger equation (2) with the effective binding potential (3). It is worth noting that in the regime \(n \gg 1\) of fast decaying inverse power-law potentials, one finds from (31) the compact formula\(^{15,16}\)

\[
\frac{2\mu\beta_r}{\hbar^2} \cdot E_{\text{max}}^{\text{max}}(n \gg 1, l)
\]

\[
= - \left\{ \frac{(-1)^l}{\pi} \left[2l + 1\right]! \left(n - 2\right)^{\frac{2l+1}{2}} \Gamma\left(\frac{2l + 1}{n - 2}\right) \right\}^2 \frac{J_l(j_{0,k})}{Y_0(j_{0,k})} \Delta_k
\]

for the characteristic threshold energy of the most excited bound-state resonance.

As a consistency check, it is worth mentioning that, in the special case of spherically symmetric (\(l = 0\)) wave functions, Eq. (24) reduces to the semi-classical result \(\kappa = 1/(a - \bar{a})\) of [12], where \(a\) is the s-wave scattering length and \(\bar{a} = \pi\rho_0(n - 2)\cot[\pi/(n - 2)]/\Gamma^2(1/(n - 2))\). In addition, it is worth emphasizing that the interesting work presented in [12] for the \(l = 0\) case is based on the semi-classical WKB analysis, whereas in the present paper we have presented a full quantum-mechanical treatment of the physical system which is valid for generic values of the dimensionless angular momentum parameter \(l\).

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\[^{14}\text{Note that this asymptotic limit corresponds to the regime in which a direct numerical integration of the Schrödinger radial equation (2) with the effective binding potential (3) becomes a non-trivial exercise.}\]

\[^{15}\text{Here we have used Eq. 6.1.34 of [13].}\]

\[^{16}\text{It is worth noting that this expression can be further simplified in the spherically symmetric (l = 0) case, in which case one finds from (32) the compact expression} \frac{2\mu\beta_n}{\hbar^2} \cdot E_{\text{max}}^{\text{max}}(n \gg 1, l) = - \left[ \frac{\pi}{\pi} \cdot \frac{\left(2\mu\beta_r\right)^{\frac{n}{n^2}}}{\hbar^2} \right]^{\frac{n}{n^2}} \cdot E_{\text{max}}^{\text{max}}(n \gg 1, l)\text{.}\]

\[^{17}\text{We would like to thank the anonymous referee for pointing out with explicit calculations this physically important fact. To see this relation, one can take} A_1 = (1 - \bar{a}/a)(n - 2)^{-11/2(n - 2)^2}\Gamma(1/(n - 2))\text{ and } A_2 = \pi\rho_0(n - 2)^{-11/2(n - 2)^2}\Gamma(1/(n - 2))\text{ in Eq. (12), where}\ \bar{a} = \pi\rho_0(n - 2)\cot[\pi/(n - 2)]/\Gamma^2(1/(n - 2)).\text{ This would yield the zero-energy} \ l = 0 \text{ asymptotic} r \rightarrow \infty \text{ solution} \psi_0(r) = 1 - r/a, \text{ where} a \text{ is the s-wave scattering length. Substituting the dimensionless ratio} A_2/A_1 = \pi/\left(\bar{a}/a\right)(n - 2)^{-11/2(n - 2)^2}\Gamma(1/(n - 2))\text{ into Eq. (24), one finds} \ \kappa = 1/(a - \bar{a})\text{ for the spherically symmetric} \ l = 0 \text{ modes, in agreement with [12].}\]

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