

Analytic solution for a class of multiscale long-range potentials

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We present a unified exact analytic solution of the radial Schrödinger equation with a class of four long-range potentials, three of which are two-scale. The physics of different potentials are encapsulated in the solution variable and parameters. Based on this solution and its asymptotic behaviors, we generalize Bo Gao's formulation of quantum defect theory for single-scale potentials to two-scale regime. As an application of this two-scale quantum defect theory, we propose a concept of harmonic oscillator quantum defect of energy levels in a spherical harmonic trap, which characterizes the effect of the two-body interactions on their trap states. This concept is a generalization of the standard quantum defect for Coulomb potential, with a distinct feature that the equations followed by the two types of quantum defects induced by the potentials under study are formally the same yet with different parameters. Examples of these two quantum defects are illustrated for Rb and Cs atoms.

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I. INTRODUCTION

Physical systems or processes are usually characterized by the scalings of certain quantities. In atomic and molecular physics, two-body interactions originating from electromagnetic forces often play the role. The interaction potentials in many cases are expressed as power-law functions of the distance r between interacting particles [1]. The name long-range potential (LP) indicates that it is valid over a large range and decays as a power law of r in the large r limit [2]. With such an LP

$$V(r) \equiv V_\alpha(r) := -\frac{C_\alpha}{r^\alpha}, \quad (1)$$

the radial Schrödinger equation (see, e.g., Refs. [2–4])

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r) - \epsilon \right] u(r) = 0 \quad (2)$$

for a two-body system has a scaling length

$$\beta_\alpha := \left(\frac{2\mu |C_\alpha|}{\hbar^2} \right)^{\frac{1}{\alpha-2}}, \quad (3)$$

where μ is the reduced mass. A Schrödinger system with one C_α in $V(r)$ is referred to a single-scale system. Examples are Coulomb potential ($\alpha = 1$) (sometimes named very-long-range potential [2]), the resonant dipole-dipole interaction ($\alpha = 3$) for collisions in a radiation field [1,5] or atom-surface

collisions [2], the polarization interaction ($\alpha = 4$) between a charged particle and a neutral particle [6–8], and the van der Waals potential (vdW) ($\alpha = 6$) between two neutral atoms at ground states [1,9]. The potential exponent α in $V(r)$ is the main character of the system [10].

However, in most cases interactions are essentially multiscale in the sense of multipole expansion. The single-scale power-law potential is the leading term of corresponding power series [1], except that for the Bohr hydrogen atom. A single-scale analysis works within certain energy scopes, where the leading power-law term dominates, otherwise a more complicated multiscale theory is required. A well-known example is the Rydberg-Ritz formula for hydrogenic atoms [11,12],

$$E_{nl} - E_i = -\frac{R_M}{(n - \mu_i^{\text{Coul}})^2}. \quad (4)$$

Although this formula has been known ever since the foundation of quantum mechanics, it was not until recently that the standard Coulomb quantum defect (CQD) μ_i^{Coul} introduced therein was theoretically understood [13].

Besides particle interactions, the external fields are usually expressed in form of power law. For example in cold-atom setups, magnetic traps and optical dipole potentials to manipulate particles are routinely approximated by harmonic potentials, which eventually manifest themselves as a quadratic term in the interaction potential $V(r)$ [3]. This means that interacting particles in external fields are intrinsically multiscale systems, and single-scale descriptions are just approximations.

Difficulties in understanding multiscale potentials may stem from the fact that exact analytic solutions (EASs) of the Schrödinger equation are rare. For single-scale cases, based on the solution for Coulomb potential, the quantum defect theory (QDT) has been established by Fano, Jungen, Greene, and

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other researchers since 1970s [14–16] and later formalized by Seaton [4]. For decades, this Coulomb QDT has been the standard systematic framework connecting the properties of Rydberg states with scattering behaviors near thresholds, as well as providing insights into atomic and molecular photoabsorption processes that involve valence electron excitations [4,17–19]. Since the late 1990s, Gao has derived the exact analytic solutions for potentials $-C_6/r^6$ [9], C_3/r^3 [5], and $-C_4/r^4$ [8] using the technique of continued fractions. In the subsequent years, he and colleagues developed an expanded quantum defect theory (eQDT) [20–22] based on these solutions. eQDT has been effectively applied to ultracold atomic collisions [23–28] and atom-ion collisions [7,29,30], including dipolar interactions [31] and Feshbach resonance [32–36]. Recently, Greene systematically summarized the latest advances in QDT, especially eQDT based on single-scale EAS [37].

Starting from these single-scale EAS theories, multiscale analysis, either approximated or exact, has been put forward. For example, Ref. [38] combined eQDT for vdW interaction at short distances with eQDT for symmetric harmonic trap at large distances and obtained the energies of two atoms in a trap, ranging from deeply bound molecular states to highly excited trap states. Reference [13] presented the first two-scale EAS for the Coulomb plus polarization potential, with which the authors expressed the CQD in eQDT formulation. Afterward, Ref. [39] developed a multichannel eQDT for a two-scale potential of vdW plus an additional $-C_8/r^8$ term and applied it to the experiment of Na-Cs multichannel interactions in an optical tweezer. Additionally, Gao presented a systematic framework of multichannel eQDT for anisotropic interactions in Ref. [40]. Likewise, an EAS for anisotropic dipole-dipole plus isotropic vdW interaction was derived in Ref. [41].

This paper is an extension of our previous work on $-C_1/r - C_4/r^4$ potential [13] to obtain a unified EAS for a class of four LPs including three two-scale potentials. Based on this EAS, we generalize eQDT for single-scale potentials to the two-scale regime. As an application of the generalized eQDT, the concept of harmonic oscillator quantum defect (HOQD), a generalization of CQD, is introduced to characterize the effect of the two-body interactions on the trap states. In Sec. II, we introduce the potentials discussed and notations used in the following. In Sec. III, we derive the EAS in detail, including the calculation technique for the characteristic exponent. The asymptotic behaviors of this EAS are discussed in Sec. IV, from which a two-scale eQDT is presented in Sec. V. As application of this two-scale eQDT, we present in Sec. VI the details of derivation for the bound state energy spectrum and that for the expression of Coulomb quantum defect. Then the concept of HOQD is proposed; details can be found in Sec. VIA. Examples of CQDs for high angular momentum states and of vdW HOQDs for S state are exhibited and briefly discussed in Sec. VIB. Conclusions are given in Sec. VII.

II. POTENTIALS

A. Notations and scalings

The radial Schrödinger equation (2) with a class of isotropic LPs $V(r)$ is solved analytically in this paper. For

single-scale LP, $V(r)$ takes the form of Eq. (1), while for two-scale ones,

$$V(r) \equiv V_{\alpha,m}(r) := -\frac{C_\alpha}{r^\alpha} - \frac{C_m}{r^m}, \quad \alpha < m. \quad (5)$$

We choose a unified length scaling β_α (3), and the energy scaling is

$$\epsilon_\alpha := \frac{\hbar^2}{2\mu\beta_\alpha^2}, \quad (6)$$

with notations of wave numbers for scattering states

$$k_s := \sqrt{\epsilon_s} = \sqrt{\frac{\epsilon}{\epsilon_\alpha}} = \sqrt{\frac{\epsilon}{\hbar^2/(2\mu\beta_\alpha^2)}}, \quad (7)$$

and for bound states

$$\kappa_s := \sqrt{-\epsilon_s} = \sqrt{-\left(\frac{\epsilon}{\epsilon_\alpha}\right)}, \quad (8)$$

where subscripts “s” represent “scaled” quantities. With this scaling, the two-scale $V_{\alpha,m}$ is expressed in the scaled form

$$V_{\alpha,m}(r_s) = -\frac{1}{r_s^\alpha} - \frac{C_{m,s}}{r_s^m}, \quad (9)$$

in which

$$C_{m,s} = \left(\frac{\beta_m}{\beta_\alpha}\right)^{m-2}. \quad (10)$$

B. Potentials in scaled form

In this paper, we derive the solutions for the following potentials:

$$V_4(r) = -\frac{C_4}{r^4}, \quad (11a)$$

$$V_{1,4}(r) = -\frac{C_1}{r} - \frac{C_4}{r^4}, \quad (11b)$$

$$V_{-2,6}(r) = \frac{\mu\omega^2}{2}r^2 - \frac{C_6}{r^6}, \quad (11c)$$

$$V_{3,4}(r) = -\frac{C_3}{r^3} - \frac{C_4}{r^4}. \quad (11d)$$

V_4 characterizes the charge-atom collisions and charge-molecule collisions [7,8]. $V_{1,4}$ is the “Coulomb + polarization” interaction that we initially discussed [13]. For two identical atoms in a harmonic trap interacting via the vdW potential, the relative motion of the system is influenced by both the interparticle interaction potential and the external trapping potential, i.e., $V_{-2,6}$ [38], which is especially interesting if the harmonic microtrap is sufficiently tight that its scaling length is comparable or almost comparable to that of the vdW potential [42]. The model potential $V_{3,4}$ is special in that both LP terms of the potential are inside the centrifugal barrier. If the C_4 takes a negative sign, potential $V_{3,4}$ belongs to the Lennard-Jones potential of the type $LJ(n, 2n-2)$ [43].

The scaled radial Schrödinger equation hereby takes a concise form

$$\left[\frac{d^2}{dr_s^2} - \frac{l(l+1)}{r_s^2} - V(r_s) + \epsilon_s \right] u(r_s) = 0, \quad (12)$$

TABLE I. Variable and parameters, in which $\tilde{w} = 2w - 1$.

Potential	$x(r_s)$	$\tilde{w}$	q
$V_4(r_s)$	$1/r_s$	0	$\sqrt{-\epsilon_s}$
$V_{1,4}(r_s)$	$\sqrt{C_{4,s}}/r_s$	$1/\sqrt{-\epsilon_s}$	$\sqrt{-\epsilon_s} C_{4,s}$
$V_{-2,6}(r_s)$	$\sqrt{C_{6,s}}/(2r_s^2)$	$\epsilon_s/2$	$\sqrt{C_{6,s}}/4$
$V_{3,4}(r_s)$	$\sqrt{\epsilon_s} r_s$	$1/\sqrt{-C_{4,s}}$	$\sqrt{-\epsilon_s} C_{4,s}$

and the four potentials discussed above have the corresponding scaled forms:

$$V_4(r_s) = -\frac{1}{r_s^4}, \quad (13a)$$

$$V_{1,4}(r_s) = -\frac{1}{r_s} - \frac{C_{4,s}}{r_s^4}, \quad (13b)$$

$$V_{-2,6}(r_s) = r_s^2 - \frac{C_{6,s}}{r_s^6}, \quad (13c)$$

$$V_{3,4}(r_s) = -\frac{1}{r_s^3} - \frac{C_{4,s}}{r_s^4}. \quad (13d)$$

III. SOLUTION

A. Change of variable and transformation

Exact analytic solution of the scaled radial Schrödinger equation (12) with four different potentials can be expressed in a unified form

$$u(r_s) = r_s^{\frac{1}{2}} e^{-\frac{q}{x(r_s)}} v(x(r_s)). \quad (14)$$

After transforming function $u(r_s)$ into $v(x)$ with proper choice of variable $x(r_s)$ and the parameter q , an equation of $v(x)$ can be deduced from Eq. (12):

$$\left[x^2 \frac{d^2}{dx^2} + x \frac{d}{dx} + (x^2 - v_0^2) + 2q \frac{d}{dx} + 2(w-1) \frac{q}{x} \right] v(x) = 0. \quad (15)$$

By the function transformation and variable changing, the differential equation of $v(x)$ with respect to x is regardless

of the potential, and the difference of physics for the four potentials is incorporated in the variable x and parameters $\{v_0, w, q\}$. The definition of v_0 follows that in Ref. [22], $v_0 := (2l+1)/(m-2)$, where the exponent m appears in Eqs. (9) and (13) (in the single-scale case $m = \alpha$), i.e., $v_0 := l + 1/2$ for potentials $V_4, V_{1,4}$, and $V_{3,4}$, while $v_0 := (l + 1/2)/2$ for $V_{-2,6}$. Other definitions are given in Table I [44].

B. Neumann expansion and general solution

The differential equation (15) is similar to Bessel's equation [45]; thus, Neumann expansion [5,9,46] is applicable. A pair of linearly independent solutions of this second-order differential equation reads

$$v^{(\pm)}(x) = \sum_{j=-\infty}^{\infty} (\pm 1)^j b_j J_{\pm(v+j)}(x), \quad (16)$$

where $J_\nu(x)$ is the Bessel function of the first kind [45]. With v taking a root of the characteristic function expressed in Sec. III C, the expansion coefficients b_j follow a series of difference equations

$$h_j^{(+)}(v) b_{j+1} + b_j + h_j^{(-)}(v) b_{j-1} = 0, \quad (17)$$

in which the function

$$h_j^{(\pm)}(v) \equiv \pm h(\pm(v+j)) \quad (18)$$

is defined by

$$h(v) := \left(\frac{q}{v^2 - v_0^2} \right) \left(\frac{v+w}{v+1} \right), \quad (19)$$

where definitions of the parameters v_0 , w , and q for different potentials are given in Table I.

The second-order difference equation (17) of b_j can be solved by the continued fraction technique [9] and the solutions are given as functions of v by

$$b_j(v) = q^j \frac{\Gamma(v)}{\Gamma(v+j)} \frac{\Gamma(v-w+1+j)}{\Gamma(v-w+1)} \frac{\Gamma(v-v_0+1+j)}{\Gamma(v-v_0+1+j)} \frac{\Gamma(v+v_0+1+j)}{\Gamma(v+v_0+1+j)} c(v+j), \quad j \geq 0, \quad (20)$$

$$b_{-j}(v) = (-q)^j \frac{\Gamma(v+1-j)}{\Gamma(v+1)} \frac{\Gamma(v+w)}{\Gamma(v+w-j)} \frac{\Gamma(v-v_0-j)}{\Gamma(v-v_0)} \frac{\Gamma(v+v_0-j)}{\Gamma(v+v_0)} c(-v+j), \quad j \geq 0, \quad (21)$$

in which $\Gamma(v)$ is the Gamma function [45] and

$$\frac{c(v+j+1)}{c(v+j)} = Q(v+j), \quad (22)$$

where the continued fraction $Q(v)$ is defined by

$$Q(v) = \frac{1}{1 + h(v+1)h(-(v+2))Q(v+1)}. \quad (23)$$

It is convenient to set $b_0 = 1$ without loss of generality, so that $c(\pm v) = 1$.

C. Root of the characteristic function

The value of v in Neumann expansion (16) is crucial in providing the starting point of the recursion, and it is the root of a characteristic function

$$\Lambda(v) := 1 + h(v)h(-v-1)Q(v) + h(-v)h(v-1)Q(-v), \quad (24)$$

which originates from the zeroth difference equation of (17) and can be obtained through the Hill determinant. This connection has been recognized by mathematicians and mathematical physicists in discussions about the Mathieu equation (see, e.g., Refs. [46,47]) and in atomic physics

was first used by Watanabe and Greene to discuss atomic polarizability in negative-ion photodetachment [6]. Later, Idziaszek *et al.* employed this mathematical relation in constructing a multichannel eQDT for ultracold atom-ion collisions [7]. Subsequently, Gao generalized it be-

yond $-1/r^4$ interaction [8,13]. We hereby present an explicit and detailed discussion of this mathematical relation.

The coefficients of the linear algebraic equations (17) define the Hill determinant $\mathcal{D}^H$:

$$\mathcal{D}^H \equiv \mathcal{D}^H(v) := \begin{vmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & h_{-2}^{(-)} & 1 & h_{-2}^{(+)} & & & 0 & \dots \\ \dots & & h_{-1}^{(-)} & 1 & h_{-1}^{(+)} & & & \dots \\ \dots & & & h_0^{(-)} & 1 & h_0^{(+)} & & \dots \\ \dots & & & & h_1^{(-)} & 1 & h_1^{(+)} & \dots \\ \dots & 0 & & & & h_2^{(-)} & 1 & h_2^{(+)} \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix}, \quad (25)$$

in which the elements are

$$h_j^{(\pm)} \equiv h_j^{(\pm)}(v). \quad (26)$$

It can be proved that $\mathcal{D}^H(v)$ is connected to $\Lambda(v)$ by [7,8,13]

$$\mathcal{D}^H(v) = \frac{\Lambda(v)}{C(v)C(-v)}, \quad (27)$$

where

$$C(v) := \prod_{j=0}^{\infty} \mathcal{Q}(v+j) = \lim_{j \rightarrow \infty} c(v+j). \quad (28)$$

The detailed derivation can be found in Appendix A. Therefore, the root of $\Lambda(v)$ is equal to that of $\mathcal{D}^H(v)$ and can be shown to satisfy the following root equation:

$$\begin{aligned} \cos 2\pi v &= 1 - 2\mathcal{D}^H(0) \sin^2 \pi v_0 \\ &= \begin{cases} 1 - 2\mathcal{D}^H(0), & v_0 = l + \frac{1}{2}, \\ 1 - \mathcal{D}^H(0), & v_0 = \frac{1}{2}(l + \frac{1}{2}). \end{cases} \end{aligned} \quad (29)$$

The details of proof are given in Appendix B.

D. Relations of the variable and parameters

To simplify the derivations, x , q , and $\tilde{w}$ are introduced in Table I in their scaled form, and we emphasize that they connect to each other and to those for other potentials [5,9]. To illustrate this explicitly, here we temporarily label them by subscripts in the same way as corresponding potentials. Noticing the definition of $x_{1,4}$ and scalings (see Sec. II A), we have

$$x_{1,4} = \frac{\sqrt{C_{4,s}}}{r_s} = \frac{\beta_4/\beta_1}{r/\beta_1} = \frac{1}{r/\beta_4} = x_4, \quad (30)$$

which means that the variable x of the solution for the potentials $V_{1,4}$ and V_4 is the same as that in Ref. [8]. Similarly,

$$x_{3,4} = \sqrt{\epsilon_s} r_s = \sqrt{\frac{\epsilon}{\hbar^2}} \frac{r}{\beta_3} = \sqrt{\frac{2\mu\epsilon}{\hbar^2}} r, \quad (31)$$

which is the same as the argument of the Neumann expansion in the solution for the potential $V_3(r)$ [5]. As for the potential

$V_{-2,6}$,

$$x_{-2,6} = \frac{\sqrt{C_{6,s}}}{2r_s^2} = \frac{(\beta_6/\beta_{-2})^2}{2(r/\beta_{-2})^2} = \frac{1}{2(r/\beta_6)^2}, \quad (32)$$

which is the same as the x of the solution for the vdW potential $V_6(r)$ in Ref. [9]. Discussions for q are similar,

$$q_{1,4} = q_{3,4} = \sqrt{-\epsilon_s C_{4,s}} = \sqrt{-\frac{\epsilon}{\epsilon_4}} = q_4, \quad (33)$$

which means that the nature of q for these three different potentials is the same in essence, whereas for $V_{-2,6}$ [cf. Eqs. (10) and (3)],

$$q_{-2,6} = \frac{\sqrt{C_{6,s}}}{4} = \frac{1}{4} \left(\frac{\beta_6}{\beta_{-2}} \right)^2 \quad (34a)$$

$$= \frac{1}{2} \frac{(\frac{1}{2}\mu\omega^2\beta_6^2)}{\hbar\omega} \quad (34b)$$

$$= \frac{1}{4} \frac{\epsilon_{-2}}{\epsilon_6}. \quad (34c)$$

As for the parameter $\tilde{w}$, we only mention that

$$\tilde{w}_{-2,6} = \frac{\epsilon_s}{2} = \frac{1}{2} \frac{\epsilon}{\epsilon_{-2}}. \quad (35)$$

Thus,

$$\frac{1}{2} \tilde{w}_{-2,6} q_{-2,6} = \frac{1}{16} \frac{\epsilon}{\epsilon_6} \quad (36)$$

is just the parameter Δ in Ref. [9].

In addition to changing variable r_s to x , another key mathematical technique is the introduction of exponential factor in the solution expression (14), the argument of which also has physical implications. For potentials V_4 and $V_{1,4}$,

$$\frac{q_{1,4}}{x_{1,4}} = \sqrt{-\epsilon_s} r_s = \frac{q_4}{x_4} = \sqrt{-1} k_s r_s, \quad (37)$$

and for $V_{3,4}$,

$$\frac{q_{3,4}}{x_{3,4}} = \sqrt{-\left(\frac{r}{\beta_4}\right)^{-2}} = \sqrt{-1} x_4, \quad (38)$$

while for $V_{-2,6}$,

$$\frac{q_{-2,6}}{x_{-2,6}} = \frac{1}{2} \left(\frac{r}{\beta_{-2}} \right)^2 = \frac{1}{2} \left(\frac{\mu\omega}{\hbar} \right) r^2, \quad (39)$$

by which one can recognize the ground-state wavefunction of the spherical harmonic oscillator in expression (14).

In summary, changing the variable of $u(r_s)$ to x together with an exponential factor to $u(r_s)$, the order of the singularity of the scaled radial Schrödinger equation (12) at the origin (also at the infinity for $V_{-2,6}$) is lowered, so that with the Neumann expansions a second-order difference equation (17) is obtained, and solved using the continued fractions. The angular momentum dependence of functions such as ν is through ν_0 , while the energy dependence is through $\{w, q\}$ for the first three LPs and that for $V_{3,4}$ through $\{x, q\}$. The variable x and parameters $\{w, q\}$, as well as the exponential factor $\exp(-q/x)$, for the four potentials are interconnected and related to the known solutions of the single-scale potentials, and their physical implications are indicated.

IV. ASYMPTOTIC BEHAVIORS

Asymptotic behaviors of solutions for the above LPs are significant in that they not only base the eQDT but also infer convergence of the Neumann expansions. To explore this, we start from the base pair of the general solution (16).

A. Asymptotic at $x \ll 1$

According to the definition of x (see Table I and discussions for x in Sec. III D), for the three potentials V_4 , $V_{1,4}$, and $V_{-2,6}$, $x \ll 1 \Leftrightarrow r_s \gg 1$, while for $V_{3,4}$, $x \ll 1 \Leftrightarrow r_s \ll 1$. With the property of the Bessel function [45]

$$J_\nu(x) \xrightarrow{x \rightarrow 0} \frac{\left(\frac{x}{2}\right)^\nu}{\Gamma(1+\nu)}, \quad (40)$$

and that of the Gamma function [45]

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin \pi x} \quad (41)$$

as well as the Stirling formula [45]

$$\Gamma(x) \xrightarrow{x \gg 1} \sqrt{2\pi} x^{x-\frac{1}{2}} e^{-x}, \quad (42)$$

straightforward derivations (given in Appendix C) lead to

$$v^{(\pm)}(x) \xrightarrow{x \ll 1} \left(\frac{x}{2q} \right)^{\pm \nu} \tilde{G}(\pm \nu) {}_1F_1 \left(1 - w \mp \nu, 1 \mp 2\nu, \frac{2q}{x} \right), \quad (43)$$

in which ${}_1F_1(a, b, z)$ is the confluent hypergeometric function [45]

$${}_1F_1(a, b, z) = \sum_{j=0}^{\infty} \frac{\Gamma(a+j)}{\Gamma(a)} \frac{\Gamma(b)}{\Gamma(b+j)} \frac{z^j}{j!} \quad (44)$$

and [48]

$$\tilde{G}(\nu) := q^\nu \frac{\Gamma(1-\nu-\nu_0)\Gamma(1-\nu+\nu_0)}{\Gamma(1-2\nu)\Gamma(1+\nu)} C(-\nu). \quad (45)$$

Hence, the base pair of the Schrödinger equation (14) has asymptotic behavior at $x \ll 1$:

$$u^{(\pm)}(x) = r_s^{\frac{1}{2}} e^{-\frac{q}{x(r_s)}} v^{(\pm)}(x) \xrightarrow{x \ll 1} \tilde{G}(\pm \nu) \times \left\{ r_s^{\frac{1}{2}} e^{-\frac{q}{x}} \left(\frac{2q}{x} \right)^{\mp \nu} {}_1F_1 \left(1 - w \mp \nu, 1 \mp 2\nu, \frac{2q}{x} \right) \right\}. \quad (46)$$

With the asymptotic properties of the confluent hypergeometric function [45],

$${}_1F_1(a, b, z) \xrightarrow{|z| \rightarrow \infty} \Gamma(b) \left\{ \frac{e^z z^{a-b}}{\Gamma(a)} + \frac{z^{-a} e^{i\pi a}}{\Gamma(b-a)} \right\},$$

$$\arg z \in \left(-\frac{\pi}{2}, \frac{3\pi}{2} \right) \quad (47)$$

one can further obtain the asymptotic expressions of the base pair of the general solution:

$$u^{(\pm)}(r_s) = r_s^{\frac{1}{2}} e^{-\frac{q}{x(r_s)}} v^{(\pm)}(x(r_s)) \xrightarrow{x \ll 1} r_s^{\frac{1}{2}} \tilde{G}(\pm \nu) \times \left\{ \frac{e^{\frac{q}{x}} \left(\frac{2q}{x} \right)^{-w}}{\Gamma(1-w \mp \nu)} + \frac{e^{-\frac{q}{x}} \left(\frac{2q}{x} \right)^{w-1}}{\Gamma(w \mp \nu)} e^{i\pi(1-w \mp \nu)} \right\}, \quad (48)$$

in which a function of ν has been introduced:

$$G(\nu) := \Gamma(1-2\nu) \tilde{G}(\nu). \quad (49)$$

This function implicitly depends on the reduced energy ϵ_s and the angular momentum l , and has played an active role in single-scale eQDT [5,9,20,22,26].

B. Asymptotic at $x \gg 1$

In a similar way, using the property of the Bessel function for large argument [45],

$$J_\nu(x) \xrightarrow{x \rightarrow \infty} \sqrt{\frac{2}{\pi x}} \cos \left(x - \frac{\pi}{2} \nu - \frac{\pi}{4} \right), \quad (50)$$

one can obtain the asymptotic behaviors of the base solution pair at $x \gg 1$:

$$u^{(\pm)}(x) \xrightarrow{x \gg 1} r_s^{\frac{1}{2}} \sum_j (\pm)^j b_j \sqrt{\frac{2}{\pi x}} \cos \left(x \mp \frac{\pi}{2} (\nu + j) - \frac{\pi}{4} \right). \quad (51)$$

Note again that for the first three LPs, $x \gg 1 \Leftrightarrow r_s \ll 1$, while for potential $V_{3,4}$, $x \gg 1 \Leftrightarrow r_s \gg 1$ (see Table I and discussions for x in Sec. III D).

V. EXPANDED QDT FORMULATION

A. Reference wavefunctions

The core of this eQDT single-channel formulation is the introduction of distinct long-range reference function pairs. The function pairs are constructed from the EAS, conform to specific boundary conditions and/or asymptotic behaviors, and are adaptable to certain physical phenomena or to facilitate discussions in a certain context. Mathematically, they are pairs of linearly independent solutions of Eq. (12) and

connected to each other pair by linear transformations. The rationale for different pairs stems from physical considerations: The physics that is straightforward to recognize or understand when using one reference pair in a certain context may be difficult to see if using another pair. All of the eQDT reference function pairs are normalized to have a Wronskian of $2/\pi$ [17,22]:

$$\mathbb{W}[f, g] := f \frac{dg}{dr_s} - \frac{df}{dr_s} g = \frac{2}{\pi}. \quad (52)$$

The base reference pair f^c and g^c are defined to have energy- and partial wave-independent asymptotic behaviors near the origin. Only f^c and g^c for the first three LPs V_4 , $V_{1,4}$, and $V_{-2,6}$ are discussed here; how to define the base pair for $V_{3,4}$ will be discussed elsewhere. The common feature of the multiscale $V_{1,4}$ and $V_{-2,6}$ is that within the centrifugal barrier they both are single-scale LPs like V_4 , which physically requires that scaling lengths of other shorter-range potentials do not overlap with them. If this requirement is satisfied, in the region $r_s \ll 1$ the two-scale LPs $V_{1,4}$ and $V_{-2,6}$ behave asymptotically in a similar way to V_4 as well as other single-scale LPs discussed in eQDT [22]. Hence, the base pair is defined as the linearly independent solutions of Eq. (12) with the following asymptotic behaviors [22]:

$$\begin{pmatrix} f^c \\ g^c \end{pmatrix} \xrightarrow{r_s \ll 1} \sqrt{\frac{2}{\pi}} \sqrt{\frac{r_s}{\varrho x}} \begin{pmatrix} \cos(x - \pi/4) \\ -\sin(x - \pi/4) \end{pmatrix}, \quad (53)$$

where $\varrho = (m-2)/2$, i.e., $\varrho = 1$ for $V_{1,4}$ (also for V_4) and $\varrho = 2$ for $V_{-2,6}$.

From the asymptotic behaviors (53) and (51) at $r_s \ll 1$ (or equivalently $x(r_s) \gg 1$) for V_4 , $V_{1,4}$, and $V_{-2,6}$, straightforward algebra arrives at the expressions of f^c and g^c for these potentials:

$$\begin{pmatrix} f^c \\ g^c \end{pmatrix} := \frac{1}{\sqrt{\varrho(X^2 + Y^2) \sin^2 \pi v}} N^c \begin{pmatrix} u^{(+)} \\ u^{(-)} \end{pmatrix}, \quad (54)$$

where the matrix N^c is defined as

$$N^c := \begin{pmatrix} \sin(\frac{\pi}{2}v - \theta) & \sin(\frac{\pi}{2}v + \theta) \\ -\cos(\frac{\pi}{2}v - \theta) & \cos(\frac{\pi}{2}v + \theta) \end{pmatrix}, \quad (55)$$

while [13]

$$X := \sum_j (-)^j b_{2j}, \quad Y := \sum_j (-)^j b_{2j+1}, \quad (56)$$

and thereby

$$\cos \theta := \frac{X}{\sqrt{X^2 + Y^2}}, \quad \sin \theta := \frac{Y}{\sqrt{X^2 + Y^2}}. \quad (57)$$

B. W^c matrix and Z^c matrix

W^c and Z^c are both 2×2 coefficient matrices that connect the base pair $\{f^c, g^c\}$ with their asymptotic behaviors at large r_s for the bound states and the scattering states, respectively [21,22]. Having defined the base pair f^c and g^c , it is straightforward to construct W^c and Z^c . Note that for potential $V_{-2,6}$, strictly speaking, there are only bound states; hence, we will only discuss the W^c matrix for it.

The asymptotic expressions of $u^{(\pm)}$ at $x \ll 1$ [i.e., $r_s \gg 1$; cf. Eq. (48)] can be reformulated as

$$\begin{pmatrix} u^{(+)}(r_s) \\ u^{(-)}(r_s) \end{pmatrix} \xrightarrow{x \ll 1} U^c \begin{pmatrix} \xi^{(+)}(x(r_s)) \\ \xi^{(-)}(x(r_s)) \end{pmatrix}, \quad (58)$$

where a reference pair $\xi^{(\pm)}$ has been introduced,

$$\begin{pmatrix} \xi^{(+)}(x(r_s)) \\ \xi^{(-)}(x(r_s)) \end{pmatrix} := r_s^{\frac{1}{2}} \left(\frac{2q}{x} \right)^{-\frac{1}{2}} \begin{pmatrix} e^{-\frac{q}{x}} \left(\frac{2q}{x} \right)^{\frac{1}{2} \tilde{w}} \\ e^{\frac{q}{x}} \left(\frac{2q}{x} \right)^{-\frac{1}{2} \tilde{w}} \end{pmatrix}, \quad (59)$$

and the matrix U^c is defined as

$$U^c := \begin{pmatrix} G(v) & 0 \\ 0 & G(-v) \end{pmatrix} \begin{pmatrix} \frac{e^{i\pi(\frac{1}{2}-v-\frac{1}{2}\tilde{w})}}{\Gamma(\frac{1}{2}-v+\frac{1}{2}\tilde{w})} & \frac{1}{\Gamma(\frac{1}{2}-v-\frac{1}{2}\tilde{w})} \\ \frac{e^{i\pi(\frac{1}{2}+v-\frac{1}{2}\tilde{w})}}{\Gamma(\frac{1}{2}+v+\frac{1}{2}\tilde{w})} & \frac{1}{\Gamma(\frac{1}{2}+v-\frac{1}{2}\tilde{w})} \end{pmatrix}. \quad (60)$$

Thus, the base pair f^c and g^c for potentials V_4 , $V_{1,4}$, and $V_{-2,6}$ has a unified asymptotic form at $r_s \gg 1$ as

$$\begin{pmatrix} f^c(r_s) \\ g^c(r_s) \end{pmatrix} \xrightarrow{r_s \gg 1} \sqrt{\frac{2}{\pi \varrho}} \tilde{W}^c \times \begin{pmatrix} \xi^{(+)}(x(r_s)) \\ \xi^{(-)}(x(r_s)) \end{pmatrix}, \quad (61)$$

in which

$$\tilde{W}^c := \sqrt{\frac{\pi}{2(X^2 + Y^2) \sin^2 \pi v}} N^c U^c. \quad (62)$$

Since the Wronskian of the pair $\xi^{(\pm)}(r_s)$ with respect to r_s is asymptotically equal to ϱ , the matrix $\tilde{W}^c$ is constrained by

$$\det(\tilde{W}^c) = 1. \quad (63)$$

The physical wavefunction is constructed from the base pair f^c and g^c by introducing a short-range K matrix K^c as in the single-scale eQDT formulation [13,22],

$$u(r_s) = f^c(r_s) - K^c g^c(r_s), \quad (64)$$

where K^c is generally energy and angular momentum dependent, $K^c \equiv K^c(\epsilon, l)$.

In eQDT, the W^c matrix is defined for bound states of single-scale LPs such as V_4 in the way like [7,8,22]

$$\begin{pmatrix} f^c \\ g^c \end{pmatrix} = W^c \begin{pmatrix} p^{(+)} \\ p^{(-)} \end{pmatrix}, \quad (65)$$

which is based on the asymptotic exponential behavior of their solutions at $r_s \gg 1$,

$$\begin{pmatrix} p^{(+)}(r_s) \\ p^{(-)}(r_s) \end{pmatrix} \xrightarrow{r_s \gg 1} \frac{1}{\sqrt{\pi \kappa_s}} \begin{pmatrix} e^{-\kappa_s r_s} \\ e^{+\kappa_s r_s} \end{pmatrix}. \quad (66)$$

Now we generalize the W^c definitions (65) and (66) to include two-scale LPs $V_{1,4}$ and $V_{-2,6}$ as well as the single-scale V_4 by using

$$\begin{pmatrix} p^{(+)}(r_s) \\ p^{(-)}(r_s) \end{pmatrix} \xrightarrow{r_s \gg 1} \sqrt{\frac{2}{\pi \varrho}} \begin{pmatrix} \xi^{(+)}(x(r_s)) \\ \xi^{(-)}(x(r_s)) \end{pmatrix} \quad (67)$$

and employ the same notations as in single-scale cases [22]:

$$W^c \equiv \begin{pmatrix} W_{f+}^c & W_{f-}^c \\ W_{g+}^c & W_{g-}^c \end{pmatrix}. \quad (68)$$

Our generalization is based on the asymptotic behaviors of $u^{(\pm)}$ at $r_s \gg 1$ (48), not only for $V_{1,4}$ in negative ϵ_s regime but also for $V_{-2,6}$ in both negative and positive ϵ_s regimes. Noticing the q/x expressions for potentials $V_{1,4}$ (37) and $V_{-2,6}$ (39) and the definition of parameter $\tilde{w}$ (see Table I in Sec. III A), one immediately has the conclusion:

$$W^c = \tilde{W}^c. \quad (69)$$

For bound states of Eq. (12), the wavefunction (64) is physically required finite at $r_s \gg 1$; hence, in view of expressions (65), (66), and (68), the requirement leads to the energy spectrum equation [13]:

$$K^c = \frac{W_{f-}^c}{W_{g-}^c}. \quad (70)$$

This equation will be intensively studied and applied to the discussions of quantum defects in the next subsection.

Similarly, the Z^c matrix in eQDT is introduced for scattering states of single-scale LPs [22]:

$$\begin{pmatrix} f^c \\ g^c \end{pmatrix} = Z^c \begin{pmatrix} s \\ c \end{pmatrix}, \quad (71)$$

so that

$$\begin{pmatrix} s(r_s) \\ c(r_s) \end{pmatrix} \xrightarrow{r_s \gg 1} \sqrt{\frac{2}{\pi k_s}} \begin{pmatrix} \sin \varphi(r_s) \\ -\cos \varphi(r_s) \end{pmatrix}, \quad (72)$$

where $\varphi(r_s) = k_s r_s - \frac{\pi}{2}l$. In this paper, we only discuss the scattering states of the potentials V_4 and $V_{1,4}$, which relate to the reference pair $\xi^{(\pm)}$ by a linear transformation. To do that, we first reformulate the pair as

$$\begin{pmatrix} \xi^{(+)}(x(r_s)) \\ \xi^{(-)}(x(r_s)) \end{pmatrix} = r_s^{\frac{1}{2}} \left(\frac{2q}{x} \right)^{-\frac{1}{2}} \times \begin{pmatrix} e^{-\sqrt{-1}\frac{\pi}{2}l} & 0 \\ 0 & e^{\sqrt{-1}\frac{\pi}{2}l} \end{pmatrix} \times \begin{pmatrix} e^{-\tilde{\varphi}(x)} \\ e^{\tilde{\varphi}(x)} \end{pmatrix}, \quad (73)$$

where

$$\begin{aligned} e^{\tilde{\varphi}(x)} &\equiv e^{(\frac{q}{x}) - \frac{\tilde{w}}{2} \ln(\frac{2q}{x}) - \sqrt{-1}\frac{\pi}{2}l} \\ &= (\sqrt{-1})^{-\frac{\tilde{w}}{2}} e^{\sqrt{-1}l[|z| + \frac{|\tilde{w}|}{2} \ln|2z| - \frac{\pi}{2}l]}, \end{aligned} \quad (74)$$

in which $z \equiv q/x = \sqrt{-1}k_s r_s$ (37). Here, we take the imaginary unit as $\sqrt{-1} \equiv i$, then it can be shown by straightforward algebra that the pair $\xi^{(\pm)}$ is related to the reference pair of scattering states by

$$\begin{pmatrix} \xi^{(+)}(x(r_s)) \\ \xi^{(-)}(x(r_s)) \end{pmatrix} = \frac{1}{\sqrt{k_s}} V^c \begin{pmatrix} \sin \phi(r_s) \\ -\cos \phi(r_s) \end{pmatrix}. \quad (75)$$

The scattering states phase $\phi(r_s)$ is a generalization of those in single-scale eQDT $\varphi(r_s)$ [22] and in Coulomb scattering [4,49]: for potential V_4

$$\phi_4(r_s) = \varphi(r_s) = k_s r_s - \frac{\pi}{2}l, \quad (76)$$

and for potential $V_{1,4}$

$$\phi_{1,4}(r_s) \equiv \varphi^{\text{Coul}}(r_s) = k_s r_s + \frac{1}{2k} \ln(2k_s r_s) - \frac{\pi}{2}l, \quad (77)$$

with φ^{Coul} the Coulomb scattering phase [49]. The linear transformation matrix V^c reads

$$V^c \equiv \sqrt{\frac{1}{2}} \begin{pmatrix} -e^{\sigma+i\frac{\pi}{4}} & -e^{\sigma-i\frac{\pi}{4}} \\ e^{-\sigma+i\frac{\pi}{4}} & -e^{-\sigma-i\frac{\pi}{4}} \end{pmatrix}, \quad (78)$$

with a scattering factor

$$\sigma := \frac{\pi}{4}|\tilde{w}| - i\frac{\pi}{2}l. \quad (79)$$

Based on this reformulation of the pair $\xi^{(\pm)}$, the scattering matrix Z^c of eQDT for V_4 and $V_{1,4}$ can be expressed as

$$Z^c \equiv \begin{pmatrix} Z_{fs}^c & Z_{fc}^c \\ Z_{gs}^c & Z_{gc}^c \end{pmatrix} = W^c V^c. \quad (80)$$

Note that Z^c is also constrained by

$$\det(Z^c) = 1. \quad (81)$$

VI. ENERGY SPECTRUM AND QUANTUM DEFECTS

A. Introduction of quantum defects

In the previous section, we have derived the W^c matrix for bound states. In the same way as in single-scale cases [8,9,22], the right-hand side of Eq. (70) defines a universal function $\chi^c(\epsilon_s)$, the expression of which can be derived from the above EAS of LPs:

$$\begin{aligned} \chi^c &\equiv \frac{W_{f-}^c}{W_{g-}^c} \\ &= \frac{R^{(-)}(v) \sin(\frac{\pi}{2}v + \theta) + M(v) \sin(\frac{\pi}{2}v - \theta)}{R^{(-)}(v) \cos(\frac{\pi}{2}v + \theta) - M(v) \cos(\frac{\pi}{2}v - \theta)}, \end{aligned} \quad (82)$$

which introduces two functions

$$M(v) := \frac{G(v)}{G(-v)} \quad (83)$$

and

$$R^{(\pm)}(v) := \frac{\Gamma(1-v \pm w)}{\Gamma(1+v \pm w)} = \frac{\Gamma(1/2-v \pm \tilde{w}/2)}{\Gamma(1/2+v \pm \tilde{w}/2)}. \quad (84)$$

In eQDT formulation, the bound spectra for any potential $\tilde{V}(r)$ that is asymptotically characterized by these LPs can be retrieved from Eq. (70), where the short-range K matrix $K^c(\epsilon_s)$ can be determined by matching the short-range wavefunction for $\tilde{V}(r)$ to Eq. (64), where $\tilde{V}(r)$ essentially becomes the LP [20,22,26]. Conversely, if (part of) energy levels can be obtained experimentally or numerically, Eq. (70) can lead to a good approximation of $K^c(\epsilon_s)$ by its discrete representation on $\chi^c(\epsilon_s)$ curves [13], as will be shown below.

In the previous paper [13], we reported that in eQDT formulation the Coulomb quantum defect can be expressed as a function of the energy and the angular momentum quantum numbers, by which good agreements with experimental data for Cs and Rb have been achieved. Here we provide detailed derivation of this equation.

From energy spectrum equation (70), one can attain [13]

$$R^{(-)}(v) = \left(\frac{K^c \cos(\frac{\pi}{2}v - \theta) + \sin(\frac{\pi}{2}v - \theta)}{K^c \cos(\frac{\pi}{2}v + \theta) - \sin(\frac{\pi}{2}v + \theta)} \right) M(v). \quad (85)$$

With help of the property of the Gamma function (41), one immediately has

$$R^{(-)}(\nu) = \frac{\sin \pi(1/2 + \nu - \tilde{w}/2)}{\sin \pi(1/2 - \nu - \tilde{w}/2)} R^{(+)}(\nu), \quad (86)$$

which means that

$$\begin{aligned} & \frac{\sin \pi(\frac{1}{2} + \nu - \frac{\tilde{w}}{2})}{\sin \pi(\frac{1}{2} - \nu - \frac{\tilde{w}}{2})} \\ &= \left(\frac{K^c \cos(\frac{\pi}{2}\nu - \theta) + \sin(\frac{\pi}{2}\nu - \theta)}{K^c \cos(\frac{\pi}{2}\nu + \theta) - \sin(\frac{\pi}{2}\nu + \theta)} \right) \frac{M(\nu)}{R^{(+)}(\nu)}, \end{aligned} \quad (87)$$

and by straightforward algebra, the left-hand side of the above equation can be simplified into

$$\frac{\sin \pi(\frac{1}{2} + \nu - \frac{\tilde{w}}{2})}{\sin \pi(\frac{1}{2} - \nu - \frac{\tilde{w}}{2})} = \frac{\cot \pi \nu + \tan \frac{\pi}{2} \tilde{w}}{\cot \pi \nu - \tan \frac{\pi}{2} \tilde{w}}. \quad (88)$$

If the right-hand side of Eq. (87) is defined as an energy-dependent function of ν ,

$$t_\epsilon(\nu) := \left(\frac{K^c \cos(\frac{\pi}{2}\nu - \theta) + \sin(\frac{\pi}{2}\nu - \theta)}{K^c \cos(\frac{\pi}{2}\nu + \theta) - \sin(\frac{\pi}{2}\nu + \theta)} \right) \frac{M(\nu)}{R^{(+)}(\nu)}, \quad (89)$$

then

$$\tan \frac{\pi}{2} \tilde{w} = - \left(\frac{1 - t_\epsilon(\nu)}{1 + t_\epsilon(\nu)} \right) \cot \pi \nu. \quad (90)$$

In the energy scaling (6), the Coulomb quantum defect (CQD) μ^{Coul} is shown to be in the form [13]

$$\kappa_s = \frac{1}{2(n - \mu^{\text{Coul}})}. \quad (91)$$

Notice that for $V_{1,4}$, $\tilde{w} = 1/\kappa_s$ (cf. Table I in Sec. III A), then we immediately reach the result reported previously [13]:

$$\tan \pi \mu^{\text{Coul}} = \left(\frac{1 - t_\epsilon(\nu)}{1 + t_\epsilon(\nu)} \right) \cot \pi \nu. \quad (92)$$

Similarly, we can also use Eq. (90) to study energy spectrum of the relative motion of two identical particles with vdW interaction in a spherical harmonic trap. We first note that the energy spectrum of a pure spherical harmonic oscillator (SHO) can be established with the energy spectrum equation (70) [38],

$$K^c = 0 = \frac{\Gamma(1 - w - \nu_0)}{\Gamma(1 - w + \nu_0)}, \quad (93)$$

which requires the argument of the Gamma function in the denominator to be a negative integer,

$$1 - w + \nu_0 = -n, \quad (94)$$

then we immediately have the energy spectrum of a pure SHO,

$$\epsilon_{\text{SHO}} = 4 \left(n + \nu_0 + \frac{1}{2} \right) = 4 \left(n + \frac{l}{2} + \frac{3}{4} \right). \quad (95)$$

Following the definition of the CQD (91), we can hereby introduce the concept of harmonic oscillator quantum defect μ^{HO} to characterize the effect of the interaction between two

identical particles on the bound states (trap states) of their relative motion in a spherical harmonic trap,

$$\epsilon_s = 4(n - \mu^{\text{HO}}), \quad (96)$$

so that for a pure SHO $\beta_6 \ll \beta_{-2}$,

$$\mu_0^{\text{HO}} = - \left(\nu_0 + \frac{1}{2} \right) = - \frac{1}{2} \left(l + \frac{3}{2} \right). \quad (97)$$

By this definition, noticing $\tilde{w} = \epsilon_s/2$ for $V_{-2,6}$ (see Table I in Sec. III A), the dependence of μ^{HO} on the energy and also on the angular momentum satisfies

$$\tan \pi \mu^{\text{HO}} = \left(\frac{1 - t_\epsilon(\nu)}{1 + t_\epsilon(\nu)} \right) \cot \pi \nu. \quad (98)$$

It is interesting that it takes the same form as CQD equation (92) for $V_{1,4}$ yet with different parameters. This feature arises from the general transformation in our unified solution, which complements the established transformation between the equation for Coulomb potential and that for SHO, and attributes to their regular energy levels that rigorously adhere to a power-law form. In the next subsection, we will discuss examples of these two quantum defects.

B. Examples of CQD and HOQD

This paper focuses on derivations of the unified solution for four LPs and generalization of eQDT formulation from single-scale potential to two-scale regime, as discussed in previous sections. Applications of this two-scale eQDT to atomic spectra of rubidium and cesium for Rydberg series of S and P states have been reported in our previous paper [13], and comparing with experimental data have exhibited satisfactory precision. Here we first present more examples of other Rydberg series in Fig. 1.

As mentioned in Sec. II B, $V_{1,4}$ characterizes how a valence electron interacts with the ionic core of the atom. In addition to Coulomb interaction, the introduction of $-C_4/r^4$ LP term minimizes the energy dependence of the quantum defects introduced in eQDT [13,22]. That is why constant values of K^c lead to good enough agreements of theoretical prediction (92) with spectrum data for S and P series of Rb and Cs [13]. This conclusion can also be drawn for electrons with large angular momentum (such as F and G states) and is well justified since their wavefunctions overlap little with that of the core and they interact mostly via $V_{1,4}$ potential, which is supported by Fig. 1(a). In the figure, we choose $K^c = -1.9965$ for F series of rubidium with $C_4 = 9.076/2$ a.u. [54] and $K^c = 0.6469$ for G series of cesium with $C_4 = 15.77/2$ a.u. [52], respectively.

As illustrated in the inset of Fig. 1(b), the D series of Cs is notable in that a peak is observed in the energy variation curve of CQD, which is confirmed in a recent experiment for ultraprecise determination of $\text{Cs}(nS_{1/2})$ and $\text{Cs}(nD_J)$ quantum defects [53]. While this nonmonotonic behavior has not been successfully explained in existing theoretical studies, it can be precisely reproduced in our two-scale eQDT with an energy-dependent K^c . As depicted in the figure, by fitting the discrete representation of K^c on the spectra to a quadratic energy-dependent $K^c(\epsilon_s) = -0.4065 - 3.0803\epsilon_s + 5.0935\epsilon_s^2$ with $C_4 = 15.77/2$ a.u., our two-scale eQDT achieves a good

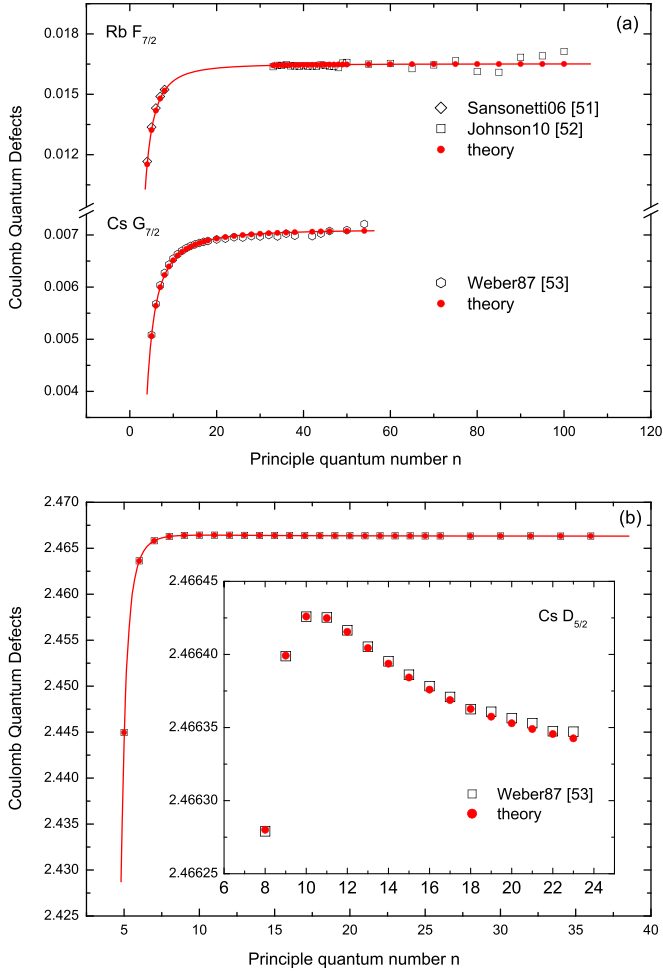


FIG. 1. Energy variation of the Coulomb quantum defects (CQDs). Red solid dots are theoretical prediction of Eq. (92) with connecting lines to guide eyes. Open symbols represent experimental data using Eq. (91). (a) CQDs for $F_{7/2}$ series of Rb with spectra data from Refs. [50] (empty diamonds) and [51] (empty squares), and those for $G_{7/2}$ series of Cs with spectra data from Ref. [52] (empty hexagons); (b) CQDs for $D_{5/2}$ series of Cs with spectra data from Ref. [52] (empty squares), and the inset is a magnification showing the nonmonotonic behavior observed also in a recent experiment [53]. See text for detailed discussions.

agreement with the experimental data [52]. The differences approach our computational precision limits.

Figures 2 and 3 are examples of HOQD μ^{HO} (96), the concept of which has been introduced in the previous subsection to characterize how the internal interaction of a dimer affects its external motions in a spherical harmonic trap. Figure 2 of vdW HOQD versus principle quantum numbers of molecular external energy levels mimics Fig. 1 of CQD versus principle quantum numbers of atomic internal energy levels. As explained above, HOQD is so defined that the vdW μ^{HO} satisfies the same equation (98) as that of CQD μ^{Coul} [Eq. (92)], and the difference of two potentials comes in through solution parameters $\{q, w, v_0\}$. Note that the red dashed line in the figure is the HOQD of the harmonic trap itself [Eq. (97)] (i.e., without the vdW interaction $C_{6,s} \approx 0$). $C_{6,s}$ characterizes the relative vdW interaction strength to the harmonic trap by

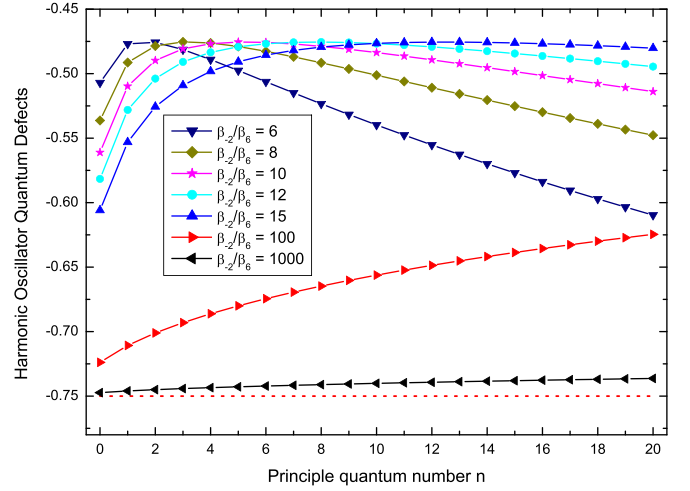


FIG. 2. Energy variation of the harmonic oscillator quantum defect [Eq. (96)], for $l = 0$. Different colors and symbols represent HOQD for different spherical harmonic trap lengths $\beta_{-2} \equiv \sqrt{\hbar/(\mu\omega)}$ relative to a fixed vdW interaction length β_6 of two identical ^{85}Rb atoms with $C_6 = 4533$ a.u. [20]. Connecting lines to guide eyes follow the analytic equation (98). A red dashed line represents that for a pure SHO [Eq. (97)] for $l = 0$ state. See text for details.

the ratio of their scaling lengths (10). For small but nonzero interaction $C_{6,s}$, HOQD is higher than μ_0^{HO} , equivalent to the lowering of the trap state energy. And the higher the energy level, the larger the vdW HOQD, as shown in the figure. With further decrease of the (relative) trap length, a peak of the HOQD curve appears, which means that for a small enough

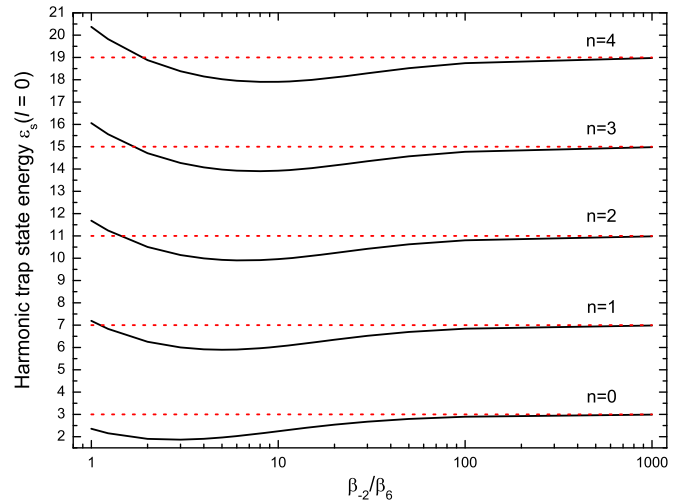


FIG. 3. Scaled energy levels (black solid lines) of trap bound states for different trap lengths relative to the vdW interaction length β_6 of two identical ^{85}Rb atoms, i.e., the eigenenergy [Eq. (82)] above the threshold of the scaled radial Schrödinger equation (12) with a two-scale potential $V_{-2,6}(r_s)$ [Eq. (13c)] for different $C_{6,s}$ [Eq. (10)], in which the length scale [Eq. (3)] is $\beta_{-2} \equiv \sqrt{\hbar/(\mu\omega)}$ and the energy scale [Eq. (6)] is $\epsilon_{-2} \equiv \hbar\omega/2$. Here we fix the vdW length with $C_6 = 4533$ a.u. for ^{85}Rb [20]. Red dashed lines represent the limit of each energy levels of $l = 0$ trap state $\epsilon_{\text{SHO}} = 4n + 3$ [Eq. (95)] for a very weak trap $\omega \sim 0$. See text for discussions.

trap length lowering trap state energy can achieve maximum at a certain medium energy level. However, Fig. 2 indicates that if the trap is too tight, the HOQD curve cannot support a peak and will become monotonically declining.

Figure 3 presents an alternative way of visualizing the interaction effect on trap states. It shows that reducing the trap length β_{-2} lowers each energy levels of the trap bound states, meaning that the attractive vdW interaction tends to *freeze* (reduce) their relative motion of the two identical particles, yet only to some extent, since there are minima in the level curves. A possible explanation is that in a tighter trap (or with stronger interaction) the external harmonic potential coalesces with the internal interaction potential, so that the positive energy levels are the extension of the molecular bound states of the combined potentials. The results in Figs. 2 and 3 are produced for ^{85}Rb . Physical parameters take the values of $C_6 = 4533$ a.u. and $K^c = 0.3106$, so that this vdW interaction supports the same number of molecular bound states as the real two-atom system of ^{85}Rb [20].

VII. CONCLUSIONS

In conclusion, we have derived an exact analytic solution in a unified form for four long-range interaction potentials, including three two-scale potentials. It is an extension and generalization of our previous work [13] with some adjustments in notation to accommodate additional potentials. The unified solution is found compact and succinct [55].

The asymptotic properties of this unified solution are deduced, and the differences in physical behavior of various potentials are incorporated in the variable and parameters of the solution. Based on the solution pair, a two-scale expanded QDT is presented, which is a generalization of the single-scale expanded QDT and may build a bridge between expanded QDT and the standard Coulomb QDT. Using this two-scale expanded QDT we have verified Seaton's theorem [2,4] by exact analytic expressions, which to our knowledge is the first rigorous verification of this theorem, and discussions in detail will be presented elsewhere.

The idea of Coulomb quantum defect is extended to the trap bound states of two interacting identical particles in a spherical harmonic trap, whence we propose a concept of harmonic oscillator quantum defect to characterize the effect of particle interactions on their trap states. The harmonic oscillator quantum defect of a van der Waals interaction $-C_6/r^6$ is found to follow the same equation as the Coulomb quantum defect of a polarization interaction. Properties of the exact solutions for the two-scale potentials, especially the van der Waals harmonic oscillator quantum defect, merit further investigation, which may provide insights into confinement-induced resonances in ultracold atoms [56,57], and may enlighten a method to measure C_6 of two-body van der Waals interaction.

Any model interaction potential, either multiscale or single-scale, is an approximation to the real interaction. In that sense, an exact analytic solution is *exact* only relatively. However, an exact analytic solution to a physical model can bring greater computing efficiency and accuracy when embedding the model into more complex systems. What underlies the unification of solutions above might imply methods toward an undiscovered classification of Lennard-Jones potentials, and provide clues to solving them in the future. Exact analytic solutions for long-range interactions, such as those presented in this paper, involve mathematics not yet extensively explored, but have convinced of their payoffs in preceding studies. What they might contribute to scattering physics and to many-body problems remains future exploration.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: PROOF OF THE RELATION BETWEEN HILL DETERMINANT AND THE CHARACTERISTIC FUNCTION

The Hill determinant has been defined in the main text [i.e., Eq. (25)] with a tridiagonal structure so that it is convenient to make algebraic expansion to it. First, we define its j th minor determinants $D_{\pm j}(\nu) \equiv D(\nu \pm (j-1)) \equiv D_{\pm j}$:

$$D_j := \begin{vmatrix} 1 & h_j^{(+)} & 0 & 0 & \cdots \\ h_{(j+1)}^{(-)} & 1 & h_{(j+1)}^{(+)} & 0 & \cdots \\ 0 & h_{(j+2)}^{(-)} & 1 & h_{(j+2)}^{(+)} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix} \quad (\text{A1})$$

and

$$D_{-j} := \begin{vmatrix} \vdots & \vdots & \vdots & \vdots \\ \cdots & h_{-(j+2)}^{(-)} & 1 & h_{-(j+2)}^{(+)} & 0 \\ \cdots & 0 & h_{-(j+1)}^{(-)} & 1 & h_{-(j+1)}^{(+)} \\ \cdots & 0 & 0 & h_{-j}^{(-)} & 1 \end{vmatrix}. \quad (\text{A2})$$

Note that based on the definition of the function $h(\nu)$ [Eqs. (18) and (19)], one can prove the relation between the two j th minor determinants:

$$D_{-j}(\nu) = D_j(-\nu). \quad (\text{A3})$$

Expanding the Hill determinant equation (25) along the zeroth row yields

$$\mathcal{D}^H = 1 \cdot T_0^{(1,0)} - h_0^{(-)} T_0^{(1,-)} - h_0^{(+)} T_0^{(1,+)}, \quad (\text{A4})$$

where the three cofactors in this first expansion of D are

$$T_0^{(1,0)} := \begin{vmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & h_{-2}^{(-)} & 1 & h_{-2}^{(+)} & & & 0 & \dots \\ \dots & & h_{-1}^{(-)} & 1 & 0 & & & \dots \\ \dots & & & 0 & 1 & h_1^{(+)} & & \dots \\ \dots & 0 & & & h_2^{(-)} & 1 & h_2^{(+)} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix}, \quad (\text{A5})$$

$$T_0^{(1,-)} := \begin{vmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & h_{-3}^{(-)} & 1 & h_{-3}^{(+)} & & & & 0 & \dots \\ \dots & & h_{-2}^{(-)} & 1 & 0 & & & & \dots \\ \dots & & & h_{-1}^{(-)} & h_{-1}^{(+)} & 0 & & & \dots \\ \dots & & & & h_1^{(-)} & 1 & h_1^{(+)} & & \dots \\ \dots & 0 & & & & h_2^{(-)} & 1 & h_2^{(+)} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix}, \quad (\text{A6})$$

$$T_0^{(1,+)} := \begin{vmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & h_{-1}^{(-)} & 1 & h_{-1}^{(+)} & & & & 0 & \dots \\ \dots & & 0 & h_1^{(-)} & h_1^{(+)} & & & & \dots \\ \dots & & & 0 & 1 & h_2^{(+)} & & & \dots \\ \dots & & & & h_3^{(-)} & 1 & h_3^{(+)} & & \dots \\ \dots & 0 & & & & h_4^{(-)} & 1 & h_4^{(+)} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix}. \quad (\text{A7})$$

Then continue to expand these cofactors and we have

$$T_0^{(1,0)} = D_{-1} D_1, \quad (\text{A8})$$

$$T_0^{(1,-)} = h_{-1}^{(+)} T_{-1}^{(2,0)} - h_{-1}^{(-)} T_{-1}^{(2,-)}, \quad (\text{A9})$$

$$T_0^{(1,+)} = h_1^{(-)} T_1^{(2,0)} - h_1^{(+)} T_1^{(2,+)}, \quad (\text{A10})$$

in which the cofactors in the expansion of $T_0^{(1,-)}$ are

$$T_{-1}^{(2,0)} := \begin{vmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & h_{-4}^{(-)} & 1 & h_{-4}^{(+)} & & & & 0 & \dots \\ \dots & & h_{-3}^{(-)} & 1 & h_{-3}^{(+)} & & & & \dots \\ \dots & & & h_{-2}^{(-)} & 1 & 0 & & & \dots \\ \dots & & & & 0 & 1 & h_1^{(+)} & & \dots \\ \dots & & & & & h_2^{(-)} & 1 & h_2^{(+)} & \dots \\ \dots & 0 & & & & & h_3^{(-)} & 1 & h_3^{(+)} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix} = D_{-2} D_1, \quad (\text{A11})$$

$$T_{-1}^{(2,-)} := \left| \begin{array}{cccc|cccc} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & h_{-4}^{(-)} & 1 & h_{-4}^{(+)} & & & 0 & \cdots \\ \cdots & & h_{-3}^{(-)} & 1 & 0 & & & \cdots \\ \cdots & & & h_{-2}^{(-)} & 0 & 0 & & \cdots \\ \cdots & & & & h_1^{(-)} & 1 & h_1^{(+)} & \cdots \\ \cdots & & & & & h_2^{(-)} & 1 & h_2^{(+)} \\ \cdots & 0 & & & & & h_3^{(-)} & 1 & h_3^{(+)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{array} \right| = 0. \quad (\text{A12})$$

Hence, the second cofactor in the first expansion (A4) is simplified into

$$T_0^{(1,-)} = h_{-1}^{(+)} D_{-2} D_1. \quad (\text{A13})$$

Similarly, the two cofactors in the expansion of $T_0^{(1,+)}$ are

$$T_1^{(2,0)} := \left| \begin{array}{cccc|cccc} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & h_{-2}^{(-)} & 1 & h_{-2}^{(+)} & & & 0 & \cdots \\ \cdots & 0 & h_{-1}^{(-)} & 1 & 0 & & & \cdots \\ \cdots & & & 0 & 1 & h_2^{(+)} & & \cdots \\ \cdots & & & & h_3^{(-)} & 1 & h_3^{(+)} & \cdots \\ \cdots & & & & & h_4^{(-)} & 1 & h_4^{(+)} \\ \cdots & 0 & & & & & h_5^{(-)} & 1 & h_5^{(+)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{array} \right| = D_{-1} D_2, \quad (\text{A14})$$

$$T_1^{(2,+)} := \left| \begin{array}{cccc|cccc} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & h_{-2}^{(-)} & 1 & h_{-2}^{(+)} & & & & \cdots \\ \cdots & & h_{-1}^{(-)} & 1 & h_{-1}^{(+)} & & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & h_2^{(+)} & & \cdots \\ \cdots & & & 0 & 1 & h_3^{(+)} & & \cdots \\ \cdots & & & & h_4^{(-)} & 1 & h_4^{(+)} & \cdots \\ \cdots & & 0 & & & h_5^{(-)} & 1 & h_5^{(+)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{array} \right| = 0. \quad (\text{A15})$$

Thus, the third cofactor in the first expansion (A4) is

$$T_0^{(1,+)} = h_1^{(-)} D_{-1} D_2. \quad (\text{A16})$$

Therefore, the expansion of the Hill determinant (A4) is simplified into the form

$$\mathcal{D}^H = D_{-1} D_1 - h_0^{(-)} h_{-1}^{(+)} D_{-2} D_1 - h_0^{(+)} h_1^{(-)} D_{-1} D_2. \quad (\text{A17})$$

Now we turn to the next level of expansion of the minor determinants $D_{\pm 1}$:

$$D_1 = D_2 - h_1^{(+)} h_2^{(-)} D_3, \quad (\text{A18})$$

$$D_{-1} = D_{-2} - h_{-1}^{(-)} h_{-2}^{(+)} D_{-3}. \quad (\text{A19})$$

One may note that these two recurrence relations are of second-order difference equation, somewhat similar to Eq. (17). Whence we introduce a notation as the ratio of the nearest two level of minors $D_{j+1}(v)$ and $D_j(v)$:

$$\mathcal{Q}^{(+)}(v+j-1) \equiv \mathcal{Q}_{j-1}^{(+)}(v) := \frac{D_{j+1}(v)}{D_j(v)}, \quad (\text{A20})$$

so that

$$\mathcal{Q}^{(+)}(v) = \mathcal{Q}_0^{(+)}(v) = \frac{D_2(v)}{D_1(v)} \quad (\text{A21})$$

and

$$\mathcal{Q}^{(+)}(v+1) = \mathcal{Q}_1^{(+)}(v) = \frac{D_3(v)}{D_2(v)}. \quad (\text{A22})$$

From the above relation of the determinants, one could reasonably infer that

$$\mathcal{Q}^{(+)}(v) = \frac{1}{1 - h_1^{(+)}(v)h_2^{(-)}(v)\mathcal{Q}^{(+)}(v+1)} = \frac{1}{1 - h^{(+)}(v+1)h^{(-)}(v+2)\mathcal{Q}^{(+)}(v+1)}. \quad (\text{A23})$$

Comparing this equation with Eq. (23), one immediately has

$$\mathcal{Q}^{(+)}(v) = \mathcal{Q}(v), \quad (\text{A24})$$

which means

$$D_2(v) = \mathcal{Q}(v)D_1(v), \quad (\text{A25})$$

then one can conclude that

$$D_1(v) \equiv D(v) = (C(v))^{-1} \equiv \left(\prod_{j=0}^{\infty} \mathcal{Q}(v+j) \right)^{-1}. \quad (\text{A26})$$

Noticing relation (A3), a similar conclusion can be drawn after same procedures:

$$D_{-1}(v) \equiv D(-v) = (C(-v))^{-1} \equiv \left(\prod_{j=0}^{\infty} \mathcal{Q}(-v+j) \right)^{-1}. \quad (\text{A27})$$

Summarizing the above results, we finally arrive at the conclusion [Eq. (27)]:

$$\mathcal{D}^H(v) = D_1(v)D_{-1}(v)[1 - h_0^{(-)}(v)h_{-1}^{(+)}(v)\mathcal{Q}(-v) - h_0^{(+)}(v)h_1^{(-)}(v)\mathcal{Q}(v)] = \frac{\Lambda(v)}{C(v)C(-v)}. \quad (\text{A28})$$

APPENDIX B: PROOF OF THE ROOT EQUATION OF THE HILL DETERMINANT

Due to the properties of the element function $h_j^{(\pm)}(v)$ [Eq. (18)] of the Hill determinant $\mathcal{D}^H(v)$ [Eq. (25)], the following mathematical conclusions about $\mathcal{D}^H(v)$ can be drawn [6–8,13,46,47]:

- (1) As a meromorphic function of v , the Hill determinant $\mathcal{D}^H(v)$ converges absolutely and uniformly except at its poles,
 - (a) $\mathcal{D}^H(v)$ is an even function with period 1;
 - (b) $n = 0, \pm 1, \dots$ are removable singularities of $\mathcal{D}^H(v)$;
 - (c) $\pm v_0 + n$ are first-order poles of $\mathcal{D}^H(v)$;
 - (d) as $\text{Im}(v) \rightarrow \pm\infty$, $\mathcal{D}^H(v) \rightarrow 1$.
- (2) The even function $\cot \pi(v - v_0) - \cot \pi(v + v_0)$ possesses the same mathematical properties (except for the absence of the removable singularity at $n = 0, \pm 1, \dots$).
- (3) Consequently, there exists a constant A such that the function

$$F(v) := \mathcal{D}^H(v) - A[\cot \pi(v - v_0) - \cot \pi(v + v_0)] \quad (\text{B1})$$

is analytic everywhere on the complex v plane and bounded as $|v| \rightarrow \infty$.

- (4) According to Liouville's theorem in complex analysis, the function $F(v)$ must be a constant $F(v) \equiv \text{const}$, and

$$\because F(v) \xrightarrow{\text{Im}(v) \rightarrow \pm\infty} 1, \quad \therefore F(v) = 1.$$

- (5) Hence,

$$\mathcal{D}^H(v) = 1 + A[\cot \pi(v - v_0) - \cot \pi(v + v_0)],$$

from which one gets

$$A = \frac{1 - \mathcal{D}^H(0)}{2 \cot \pi v_0}. \quad (\text{B2})$$

- (6) Then straightforward algebra leads to the root equation (29) for the Hill determinant $\mathcal{D}^H(v)$.

APPENDIX C: DERIVATION OF THE ASYMPTOTIC AT $x \ll 1$

Using the property of the Bessel function [45],

$$J_\nu(x) \xrightarrow{x \rightarrow 0} \left(\frac{x}{2} \right)^\nu / \Gamma(1 + \nu), \quad (\text{C1})$$

we have

$$\sum_{j=-\infty}^{\infty} b_j J_{\nu+j}(x(r_s)) \xrightarrow{x \rightarrow 0} \left(\sum_{j=-\infty}^0 + \sum_{j=1}^{\infty} \right) b_j \frac{\left(\frac{1}{2}x\right)^{\nu+j}}{\Gamma(1+\nu+j)} \xrightarrow{x \rightarrow 0} \sum_{j=0}^{\infty} b_{-j} \frac{\left(\frac{1}{2}x\right)^{\nu-j}}{\Gamma(1+\nu-j)}. \quad (\text{C2})$$

Inserting the expression of b_j and employing the property of Gamma function (41), one can obtain

$$\begin{aligned} \sum_{j=-\infty}^{\infty} b_j J_{\nu+j}(x(r_s)) &\xrightarrow{x \rightarrow 0} \left(\frac{2q}{x}\right)^{-\nu} \left\{ q^{\nu} \frac{\Gamma(1-\nu-\nu_0)\Gamma(1-\nu+\nu_0)}{\Gamma(1+\nu)} \right\} \\ &\times \sum_{j=0}^{\infty} \frac{\Gamma(1-\nu-w+j)}{\Gamma(1-\nu-w)} \frac{c(-\nu+j)}{\Gamma(1-\nu+\nu_0+j)\Gamma(1-\nu+\nu_0+j)} \left(\frac{2q}{x}\right)^j. \end{aligned} \quad (\text{C3})$$

For $x \ll 1$, important terms in the sum are those with $j \gg 1$ [9]; hence, with the Stirling formula (42) and noticing

$$(1-\nu-\nu_0+j)^{(1-\nu-\nu_0+j)-\frac{1}{2}} (1-\nu+\nu_0+j)^{(1-\nu+\nu_0+j)-\frac{1}{2}} \xrightarrow{j \gg 1} (1-2\nu+j)^{(1-2\nu+j)-\frac{1}{2}} (1+j)^{(1+j)-\frac{1}{2}}, \quad (\text{C4})$$

we have

$$\Gamma(1-\nu-\nu_0+j)\Gamma(1-\nu+\nu_0+j) \xrightarrow{j \gg 1} \Gamma(1-2\nu+j)\Gamma(1+j). \quad (\text{C5})$$

After all these approximations, the asymptotic behavior of $u^{(+)}(x(r_s))$ at $x \ll 1$ can be found:

$$\begin{aligned} u^{(+)}(x) &\xrightarrow{x \ll 1} r^{\frac{1}{2}} e^{-\frac{q}{x}} \left(\frac{2q}{x}\right)^{-\nu} \left\{ q^{\nu} \frac{\Gamma(1-\nu-\nu_0)\Gamma(1-\nu+\nu_0)}{\Gamma(1+\nu)} \right\} \sum_{j=0}^{\infty} \frac{\Gamma(1-\nu-w+j)}{\Gamma(1-\nu-w)} \frac{c(-\nu+j)}{\Gamma(1-2\nu+j)\Gamma(1+j)} \left(\frac{2q}{x}\right)^j \\ &\approx r^{\frac{1}{2}} e^{-\frac{q}{x}} \left(\frac{2q}{x}\right)^{-\nu} \tilde{G}(\nu) {}_1F_1\left(1-w-\nu, 1-2\nu, \frac{2q}{x}\right). \end{aligned} \quad (\text{C6})$$

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