General form of the quantum-defect theory for $-1/r^\alpha$ type of potentials with $\alpha>2$

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We present a general formulation of the quantum-defect theory for systems with an attractive $1/r^\alpha$ type of asymptotic potentials with $\alpha>2$. Its structural differences from the standard theory for $\alpha\leq 2$, or from the semiclassical theory, is fully explained through a systematic understanding of quantum reflection above the threshold, and quantum connection formulas below the threshold.

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I. INTRODUCTION

Through the works of many people, such as Seaton, Fano, and Greene, the quantum-defect theory (QDT) for $-1/r^\alpha$ type of potentials with $\alpha\leq 2$ has been well established as a powerful conceptual and computational tool for all physical processes that are governed by such long-range interactions [1–5]. The same cannot yet be said, however, about the QDT for interactions with $\alpha>2$, despite many important individual advances [6–15], especially since the emergence of cold-atom physics [16–29]. The reason is an intertwining combination of conceptual, mathematical, and computational difficulties.

As an example of the mathematical and related computational difficulties, consider the case of a polarization potential of the type of $-1/r^4$ that plays an important role in our understanding of electron-atom and ion-atom interactions. It has been known for years [6,30] that solutions for this potential are given by the Mathieu functions [31]. But because of the difficulties associated with understanding and computing such functions, it was not until much later [8,9,14,32–35] that this analytic solution for $-1/r^4$ provided us with more than the threshold behavior [6,36]. The solutions for all other potentials with $\alpha>2$ [19,21] are of comparable difficulty. They all belong to a class of special functions that, for nonzero energies, are solutions of second-order ordinary differential equations with two irregular singularities, one at the origin and one at infinity.

As an example of the conceptual difficulties, and also to motivate our study in this work, recall that one of the hallmark results of the QDT for $\alpha\leq 2$ can be expressed in terms of the K matrix as follows [1–4]:

$$K_l=\tan\,\delta_l=\tan(\delta_l^{(l)}+\delta_l^{(s)}). \tag{1}$$

Namely, the total scattering phase shift is a sum of a phase shift due to the long-range potential, $\delta_l^{(l)}$, which has strong energy dependence, and a phase shift due to short-range interactions, $\delta_l^{(s)}$, which depends weakly on energy and can be extrapolated across the threshold [1–4]. The comparable result that we have derived for $\alpha>2$ [19–21,23,25] takes the form

$$K_l=\tan\,\delta_l=(Z_{gc}^c K^c-Z_{fc}^c)(Z_{fs}^c-Z_{gs}^c K^c)^{-1}, \tag{2}$$

where K^c is a short-range K matrix that depends weakly on energy and can be written in terms of a short-range phase shift as $K^c=\tan\,\delta^s$. The Z_{xy}^c are elements of a 2×2 Z^c matrix that satisfies $\det(Z^c)=1$ [23]. They are all universal functions of a scaled energy that are determined solely by the long-range potential. A similar result also appears in the works of O'Malley *et al.* [6] and Cavagnero [15], and has been especially fully developed by Fabrikant for electron-atom scattering [10,13]. Equation (2) cannot generally be written in the form of Eq. (1). Furthermore, it implies that we need generally three independent functions of energy, as opposed to a single $\delta_l^{(l)}$, to characterize the effect of long-range interaction on the scattering process.

Equation (1) is so simple, and it make so much sense intuitively, that it is ingrained in our understanding of the QDT. In comparison, Eq. (2), which is structurally different from Eq. (1) as it requires three independent functions, looks suspiciously complicated. This, and other related structural differences between QDT for $\alpha>2$ and that for $\alpha\leq 2$, have been the results of mathematical derivations, but the origin of such differences has not been fully explained or understood. This lingering question about our theory, and the related question of whether it is in its most optimal form, has slowed the pace of its development considerably.

The goal of this paper is to put the QDT for $\alpha>2$, especially conceptually, on the same solid footing as that for $\alpha\leq 2$. It would be a success if at the end of this paper one were to learn to take Eq. (2) for granted, while viewing Eq. (1) as one of its special cases, in the following sense. The description of the propagation of a Schrödinger wave in one dimension generally requires three parameters; they can be reduced to a single phase shift when and only when there is no quantum reflection (see, e.g., [37–40]) by the long-range potential. This, and related physics below the threshold, are what we hope will transpire in this paper.

We start in Sec. II by briefly reviewing the characteristics of the Schrödinger equation for $-1/r^\alpha$ type of potentials. In Sec. III, we define various reference functions that are useful in QDT for $\alpha>2$, and we relate them to a base pair f^c and g^c. In particular, we will define two sets of outgoing and incoming wave-function pairs, one for the inner region and one for the outer region. They are used in Sec. IV to develop a systematic understanding of quantum reflection by and quantum transmission and tunneling through the long-range potential. In Sec. V, we discuss what we call the quantum connection formulas, in order to understand the structure of the QDT for negative energies. In Sec. VI, we define various short-range parameters including the quantum defect and a short-range S matrix. The theory is applied to reexamine the two-body

scattering process in Sec. VII, in both the K matrix and the S matrix formulations. The theory for bound states is reformulated in Sec. VIII, where we also introduce a generalized K matrix for negative energies that is useful beyond the standard two-body problem. Conclusions are given in Sec. IX. Appendix A summarizes the Z^c and W^c matrices for $\alpha=6$. Appendix B gives a semiclassical theory for the relevant QDT functions. There are two other Appendixes that expand on the discussions in the main text.

II. CHARACTERISTICS OF $-1/r^\alpha$ POTENTIALS

Consider the radial Schrödinger equation for potential $-C_\alpha/r^\alpha$, with $C_\alpha>0$ and $0<\alpha<\infty$,

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2\mu r^2}-\frac{C_\alpha}{r^\alpha}-\epsilon\right)v_{\epsilon l}(r)=0. \tag{3}$$

The special scale-invariant case of $\alpha=2$ can be easily dealt with through a redefinition of l [1,2]. For any other cases of $\alpha\neq 2$, the potential $-C_\alpha/r^\alpha$ has associated with it a length scale β_α, defined by

$$\beta_\alpha \equiv (2\mu C_\alpha/\hbar^2)^{1/(\alpha-2)}, \tag{4}$$

and a corresponding energy scale $s_E=(\hbar^2/2\mu)(1/\beta_\alpha)^2$. The scaled version of Eq. (3) takes the dimensionless form of

$$\left(\frac{d^2}{dr_s^2}-\frac{l(l+1)}{r_s^2}+\frac{1}{r_s^\alpha}+\epsilon_s\right)v_{\epsilon_s l}(r_s)=0, \tag{5}$$

where $r_s=r/\beta_\alpha$ is a scaled radius and $\epsilon_s=\epsilon/s_E$ is a scaled energy. For $l\neq 0$, the scaled effective potential $U_s(r_s)=-1/r_s^\alpha+l(l+1)/r_s^2$ has a maximum for $\alpha>2$ and a minimum for $\alpha<2$. The maximum corresponds to a potential barrier with a scale height of

$$H_{sl}=[(\alpha-2)/\alpha](2/\alpha)^{2/(\alpha-2)}[l(l+1)]^{\alpha/(\alpha-2)}. \tag{6}$$

The minimum corresponds to a potential well with a depth of $-H_{sl}$.

Equation (5) has the following characteristics. For $\alpha>2$ and $\epsilon_s\neq 0$, both $r_s=0$ and $r_s=\infty$ are irregular singularities. For $\alpha>2$ and $\epsilon_s=0$, $r_s=0$ is an irregular singularity but $r=\infty$ is a regular singularity. For $\alpha<2$, $r_s=0$ is a regular singularity and only $r_s=\infty$ is an irregular singularity. All cases of a single irregular singularity, namely $\alpha<2$, or $\alpha>2$ but $\epsilon_s=0$, can be easily solved by using, e.g., a series expansion around the regular singularity. All cases of two irregular singularities, namely $\alpha>2$ and $\epsilon_s\neq 0$, are considerably more difficult [8,14,15,19,21].

Focusing on the case of $\alpha>2$ and $\epsilon_s\neq 0$, the solution of Eq. (5) is not necessarily difficult for all energies or for all regions of space. Defining

$$k_s(r_s)\equiv\left(\epsilon_s+\frac{1}{r_s^\alpha}-\frac{l(l+1)}{r_s^2}\right)^{1/2}, \tag{7}$$

and using the criteria for the applicability of the semiclassical approximation (see, e.g., Ref. [41]),

$$\left|\frac{d}{dr_s}\frac{1}{k_s(r_s)}\right|\ll 1, \tag{8}$$

one can easily show that the semiclassical approximation is rigorously applicable (not an approximation) in three limits: (a) the limit of $|\epsilon_s|\to\infty$, namely for energies, both positive and negative, sufficiently away from the threshold; (b) the limit of $r_s\to 0$ for all energies; and (c) the limit of $r_s\to\infty$ for all energies except zero. In other words, the real difficult solutions correspond to a range of energies around the threshold, and a region in space around $r_s\sim 1$, namely $r\sim\beta_\alpha$, where the semiclassical approximation breaks down. The existence of such a regime and some of its consequences are now well known [16,17,22,42–48]. Some physical understanding of the quantum regime above the threshold have also been developed by Ward and Macek [35] for $-1/r^4$ interaction, and by Coté *et al.* [49] for ultracold s-wave atomic collisions $(-1/r^6)$. This work shows how different behaviors in the quantum and semiclassical regimes are reflected in the structure of QDT for $\alpha>2$. It gives a complete characterization of both regimes, both above and below the threshold, and for arbitrary angular momentum l.

III. PURE LONG-RANGE REFERENCE WAVE FUNCTIONS

A pure long-range reference function pair is defined as a pair of linearly independent solutions of Eq. (5). Since a second-order ordinary differential equation has only two linearly independent solutions, we need, in principle, only a single pair. (Let us call it the base pair.) All other choices of reference pairs can be related to the base pair by a linear transformation, namely by a 2×2 matrix.

The rationale for defining and using different reference pairs is thus not in math or in computation, as all physical observables can be computed using a single pair. The purpose is physical understanding. The physics that is straightforward to recognize or understand using one reference pair may be very difficult or impossible to see in another.

In all our definitions of reference pairs to follow, the Wronskian for a pair is defined with derivatives being with respect to the scaled radius r_s, e.g.,

$$W(f^c,g^c)\equiv f^c\frac{dg^c}{dr_s}-\frac{df^c}{dr_s}g^c=2/\pi. \tag{9}$$

Furthermore, all reference pairs are normalized such that they have a Wronskian of $2/\pi$. We also point out in advance that for every pair of standing-wave reference functions, there is a corresponding definition of a K matrix. And for every pair of traveling-wave reference functions, there is a corresponding definition of an S matrix. They will be discussed later in Secs. VI and VII.

A. f^c and g^c

The f^c and g^c functions form the base pair upon which many of our QDT parameters and functions are defined. They are chosen to have not only energy-independent, but also angular-momentum-independent behaviors near the ori-

gin [25]. Specifically, they are defined as the solutions of Eq. (5) with the following asymptotic behavior:

$$f^c_{\epsilon_s l}(r_s) \overset{r_s\to 0}{\sim} (2/\pi)^{1/2} r_s^{\alpha/4} \cos(y-\pi/4), \tag{10}$$

$$g^c_{\epsilon_s l}(r_s) \overset{r_s\to 0}{\sim} -(2/\pi)^{1/2} r_s^{\alpha/4} \sin(y-\pi/4) \tag{11}$$

for all energies. Here $y=[2/(\alpha-2)]r_s^{-(\alpha-2)/2}$. The normalizations have been chosen so that $W(f^c,g^c)=2/\pi$. Such solutions of Eq. (5) exist for all $\alpha>2$.

At zero energy, the solutions f^c and g^c can be easily found for arbitrary α and l [6,25]. They are given by

$$f^c_{\epsilon_s=0 l}(r_s) = [2/(\alpha-2)]^{1/2} r_s^{1/2} [J_{\nu_0}(y)\cos(\pi\nu_0/2) - Y_{\nu_0}(y)\sin(\pi\nu_0/2)], \tag{12}$$

$$g^c_{\epsilon_s=0 l}(r_s) = -[2(\alpha-2)]^{1/2} r_s^{1/2} [J_{\nu_0}(y)\sin(\pi\nu_0/2) + Y_{\nu_0}(y)\cos(\pi\nu_0/2)], \tag{13}$$

where $\nu_0=(2l+1)/(\alpha-2)$.

For nonzero energies, the solutions f^c and g^c are generally much more difficult to find [8,14,15,19,21]. Whatever they are, however, their asymptotic behaviors at large r_s can always be written, for $\epsilon_s>0$, as

$$f^c_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} \sqrt{\frac{2}{\pi k_s}}\left[Z^c_{fs}(\epsilon_s,l)\sin\left(k_s r_s - \frac{l\pi}{2}\right) - Z^c_{fc}(\epsilon_s,l)\cos\left(k_s r_s - \frac{l\pi}{2}\right)\right], \tag{14}$$

$$g^c_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} \sqrt{\frac{2}{\pi k_s}}\left[Z^c_{gs}(\epsilon_s,l)\sin\left(k_s r_s - \frac{l\pi}{2}\right) - Z^c_{gc}(\epsilon_s,l)\cos\left(k_s r_s - \frac{l\pi}{2}\right)\right], \tag{15}$$

where $k_s=\epsilon_s^{1/2}$, and can be written, for $\epsilon<0$, as

$$f^c_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} (\pi\kappa_s)^{-1/2}[W^c_{f+}(\epsilon_s,l)e^{-\kappa_s r_s} + W^c_{f-}(\epsilon_s,l)e^{+\kappa_s r_s}], \tag{16}$$

$$g^c_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} (\pi\kappa_s)^{-1/2}[W^c_{g+}(\epsilon_s,l)e^{-\kappa_s r_s} + W^c_{g-}(\epsilon_s,l)e^{+\kappa_s r_s}], \tag{17}$$

where $\kappa_s=(-\epsilon_s)^{1/2}$.

Equations (14)–(17) define a 2×2 $Z^c(\epsilon_s,l)$ matrix and a 2×2 $W^c(\epsilon_s,l)$ matrix:

$$Z^c \equiv \begin{pmatrix} Z^c_{fs} & Z^c_{fc} \\ Z^c_{gs} & Z^c_{gc} \end{pmatrix}, \tag{18}$$

$$W^c \equiv \begin{pmatrix} W^c_{f+} & W^c_{f-} \\ W^c_{g+} & W^c_{g-} \end{pmatrix}, \tag{19}$$

both of which are universal functions of the scaled energy ϵ_s and the angular momentum l that are uniquely determined by α. The Z^c matrix describes, for positive energies, the propagation of a wave function in a $-1/r^\alpha$ type of potential from small to large distances, and vice versa. The W^c matrix describes the same physics for negative energies. The full implications of these statements will become increasingly clear as the paper progresses.

Without actually solving any equation or invoking any properties of a specific potential, there are a couple of things that we do know about the Z^c and W^c matrices. First, they are both real, because Eq. (5) is real (we restrict ourselves to real energies and real angular momenta in this paper) and the boundary conditions we use to define f^c and g^c are real. Second, since the Schrödinger equation preserves the Wronskian, the Wronskian of f^c and g^c that we evaluate using their asymptotic behaviors at infinity must be equal to that obtained using Eqs. (10) and (11), which is $2/\pi$. This means that the elements of the Z^c and the W^c are not all independent, but are constrained by

$$\det(Z^c) = Z^c_{fs}Z^c_{gc} - Z^c_{gs}Z^c_{fc} = 1, \tag{20}$$

$$\det(W^c) = W^c_{f+}W^c_{g-} - W^c_{g+}W^c_{f-} = 1. \tag{21}$$

In other words, both Z^c and W^c have only three independent real elements. The same consideration and conclusion can in fact be put in a much broader context. Namely, the description of the propagation of a Schrödinger wave in one dimension generally requires three independent real parameters, an almost trivial fact, but nevertheless worth keeping in mind. The Z^c and W^c matrices for $\alpha=6$ [23,50] are summarized in Appendix A.

There is one more important property of f^c and g^c that should be noted. That is, because the boundary conditions we use to define them are independent of both ϵ_s and l, then for $\alpha>3$, f^c and g^c are entire functions of both ϵ_s and l at any finite r_s. This is due to a theorem by Poincaré [51] (see, e.g., Ref. [52]).

B. f^{c0} and g^{c0}

The reference pair of f^{c0} and g^{c0} is defined with boundary conditions near the origin that differ from those for f^c and g^c by a phase of $\pi\nu_0/2$,

$$f^{c0}_{\epsilon_s l}(r_s) \overset{r_s\to 0}{\sim} (2/\pi)^{1/2} r_s^{\alpha/4} \cos(y-\pi\nu_0/2-\pi/4), \tag{22}$$

$$g^{c0}_{\epsilon_s l}(r_s) \overset{r_s\to 0}{\sim} -(2/\pi)^{1/2} r_s^{\alpha/4} \sin(y-\pi\nu_0/2-\pi/4). \tag{23}$$

They are obviously related to f^c and g^c by an orthogonal transformation,

$$\begin{pmatrix} f^{c0} \\ g^{c0} \end{pmatrix} = \begin{pmatrix} \cos(\pi\nu_0/2) & -\sin(\pi\nu_0/2) \\ \sin(\pi\nu_0/2) & \cos(\pi\nu_0/2) \end{pmatrix} \begin{pmatrix} f^{c} \\ g^{c} \end{pmatrix}. \tag{24}$$

This pair differs only by normalization constants from the f^0 and g^0 pair used in our original solution for the $-1/r^6$ potential [19]. The K matrix defined using this pair (see Sec. VI) is still the most convenient for describing the threshold behavior [20] and cases in which either a bound state or a shape resonance state is very close to the threshold [23,28].

C. f^{i+} and f^{i-}

There are two sets of outgoing and incoming waves that can be rigorously defined for $-1/r^\alpha$ types of potentials with $\alpha > 2$. Their definitions are the key for a systematic understanding of quantum reflection by and quantum transmission and tunneling through such potentials.

f^{i+} and f^{i-} define the outgoing and incoming waves in the inner region of $r_s \ll 1$, namely $r \ll \beta_\alpha$. Specifically, they are defined by

$$f^{i+}_{\epsilon_s l}(r_s) \overset{r_s\to 0}{\sim} \frac{1}{\sqrt{\pi}} e^{i\pi/4} r_s^{\alpha/4} \exp[-i(y-\pi/4)], \tag{25}$$

$$f^{i-}_{\epsilon_s l}(r_s) \overset{r_s\to 0}{\sim} \frac{1}{\sqrt{\pi}} e^{i\pi/4} r_s^{\alpha/4} \exp[+i(y-\pi/4)], \tag{26}$$

and correspond to traveling waves with a flux of $\hbar/(\pi\mu\beta_\alpha)$ in the $\pm\hat{r}$ directions, respectively. Note that it is the negative exponential that corresponds to the outgoing wave since y is a decreasing function of r_s.

This pair is related to f^c and g^c by a unitary transformation,

$$\begin{pmatrix} f^{i+} \\ f^{i-} \end{pmatrix} = \frac{e^{i\pi/4}}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \begin{pmatrix} f^{c} \\ g^{c} \end{pmatrix}, \tag{27}$$

and similar to f^c and g^c, they are well defined by the same boundary conditions for all energies.

D. f^{o+} and f^{o-}

The previous three reference pairs are all defined with the boundary condition at small r_s. Now we discuss reference functions that are defined by their asymptotic behaviors at large r_s. These functions are used in definitions of the K and the S matrices that are closely related to the scattering experiment.

We start with f^{o+} and f^{o-}, which correspond to outgoing and incoming waves in the outer region of $r_s \gg 1$ $(r \gg \beta_\alpha)$. They are defined for positive energies by

$$f^{o+}_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} \frac{1}{\sqrt{\pi k_s}} e^{i\pi/4} \exp(+ik_s r_s), \tag{28}$$

$$f^{o-}_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} \frac{1}{\sqrt{\pi k_s}} e^{i\pi/4} \exp(-ik_s r_s), \tag{29}$$

corresponding to traveling waves with a flux of $\hbar/(\pi\mu\beta_\alpha)$ in the $\pm\hat{r}$ directions, respectively. They are defined for negative energies by

$$f^{o+}_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} \frac{1}{\sqrt{\pi\kappa_s}} \exp(-\kappa_s r_s), \tag{30}$$

$$f^{o-}_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} \frac{1}{\sqrt{\pi\kappa_s}} \exp(+\kappa_s r_s). \tag{31}$$

The phase factors and normalizations are chosen here such that (a) Eqs. (30) and (31) are analytic continuation of Eqs. (28) and (29) on the physical sheet, on which $(\epsilon_s)^{1/2} = i\kappa_s$ for negative energies. This allows for a consistent definition of the S matrix for both positive and negative energies (and also for complex energies). (b) f^{o+} and f^{o-} are both real for negative energies, while maintaining the standard definition of the S matrix for positive energies. (c) $W(f^{o+}, f^{o-}) = 2/\pi$.

Like any other solutions of Eq. (5), f^{o+} and f^{o-} can be written as linear superpositions of f^c and g^c. From Eqs. (16) and (17), it is clear that they are related, for negative energies, by the W^c matrix,

$$\begin{pmatrix} f^{c} \\ g^{c} \end{pmatrix} = W^c \begin{pmatrix} f^{o+} \\ f^{o-} \end{pmatrix} = \begin{pmatrix} W^c_{f+} & W^c_{f-} \\ W^c_{g+} & W^c_{g-} \end{pmatrix} \begin{pmatrix} f^{o+} \\ f^{o-} \end{pmatrix}, \tag{32}$$

or its inverse,

$$\begin{pmatrix} f^{o+} \\ f^{o-} \end{pmatrix} = \begin{pmatrix} W^c_{g-} & -W^c_{f-} \\ -W^c_{g+} & W^c_{f+} \end{pmatrix} \begin{pmatrix} f^{c} \\ g^{c} \end{pmatrix}. \tag{33}$$

Equation (32) explains the notation that we have chosen for the elements of the W^c matrix.

For positive energies, it is easy to show from Eqs. (14) and (15) that f^{o+} and f^{o-} are related to the base pair by

$$\begin{pmatrix} f^{o+} \\ f^{o-} \end{pmatrix} = \frac{e^{il\pi/2 - i\pi/4}}{\sqrt{2}} \begin{pmatrix} -(Z^c_{gc} - iZ^c_{gs}) & (Z^c_{fc} - iZ^c_{fs}) \\ (-1)^l (Z^c_{gc} + iZ^c_{gs}) & -(-1)^l (Z^c_{fc} + iZ^c_{fs}) \end{pmatrix} \times \begin{pmatrix} f^{c} \\ g^{c} \end{pmatrix}. \tag{34}$$

Here we have used the fact that l is an integer.

In addition to these transformations between $f^{o\pm}$ and the base pair f^c and g^c, another important set of transformations are those between $f^{o\pm}$ and $f^{i\pm}$, which, as will become clear in Secs. IV and V, are most closely related to the physics of quantum reflection above the threshold and quantum connection formulas below the threshold. Combining Eq. (34) with Eq. (27), we have for positive energies

$$\begin{pmatrix} f^{o+} \\ f^{o-} \end{pmatrix} = U^{(oi)} \begin{pmatrix} f^{i+} \\ f^{i-} \end{pmatrix} = \begin{pmatrix} U^{(oi)}_{++} & U^{(oi)}_{+-} \\ U^{(oi)}_{-+} & U^{(oi)}_{--} \end{pmatrix} \begin{pmatrix} f^{i+} \\ f^{i-} \end{pmatrix}, \tag{35}$$

where

$$U^{(oi)}_{++} = -e^{il\pi/2}[(Z^c_{fc} - Z^c_{gs}) - i(Z^c_{fs} + Z^c_{gc})]/2,$$

$$U^{(oi)}_{+-} = e^{il\pi/2}[(Z^c_{fc} + Z^c_{gs}) - i(Z^c_{fs} - Z^c_{gc})]/2,$$

$$U_{-+}^{(oi)} = (U_{+-}^{(oi)})^*,$$

$$U_{--}^{(oi)} = (U_{++}^{(oi)})^*.$$

The inverse of this transformation is

$$\begin{pmatrix} f^{i+} \\ f^{i-} \end{pmatrix} = \begin{pmatrix} (U_{++}^{(oi)})^* & -U_{+-}^{(oi)} \\ -(U_{+-}^{(oi)})^* & U_{++}^{(oi)} \end{pmatrix} \begin{pmatrix} f^{o+} \\ f^{o-} \end{pmatrix}. \tag{36}$$

From Eqs. (32) and (27), we have for negative energies

$$\begin{pmatrix} f^{o+} \\ f^{o-} \end{pmatrix} = \frac{e^{-i\pi/4}}{\sqrt{2}} \begin{pmatrix} W_{g-}^c + iW_{f-}^c & W_{g-}^c - iW_{f-}^c \\ -(W_{g+}^c + iW_{f+}^c) & -(W_{g+}^c - iW_{f+}^c) \end{pmatrix} \begin{pmatrix} f^{i+} \\ f^{i-} \end{pmatrix}. \tag{37}$$

E. s, c, $\tilde{s}$, and $\tilde{c}$

The reference pair s and c is defined for positive energies by

$$s_{\epsilon_s l}(r_s) \overset{r\to\infty}{\sim} \sqrt{\frac{2}{\pi k_s}} \sin(k_s r_s - l\pi/2), \tag{38}$$

$$c_{\epsilon_s l}(r_s) \overset{r\to\infty}{\sim} -\sqrt{\frac{2}{\pi k_s}} \cos(k_s r_s - l\pi/2). \tag{39}$$

They are normalized such that $W(s,c)=2/\pi$. Their relationship to f^c and g^c takes a simple form, from Eqs. (14) and (15), of

$$\begin{pmatrix} f^c \\ g^c \end{pmatrix} = Z^c \begin{pmatrix} s \\ c \end{pmatrix} = \begin{pmatrix} Z_{fs}^c & Z_{fc}^c \\ Z_{gs}^c & Z_{gc}^c \end{pmatrix} \begin{pmatrix} s \\ c \end{pmatrix} \tag{40}$$

for positive energies. This equation explains the notation that we have newly adopted for the elements of the Z^c matrix.

For negative energies, the analytic continuations of s and c are trivially complex by different phase factors, which also makes the corresponding K matrix imaginary. Instead of such a definition, we find it more useful to define a different pair

$$\tilde{s}_{\epsilon_s l}(r_s) \overset{r\to\infty}{\sim} \frac{1}{\sqrt{2\pi\kappa_s}} [e^{-\kappa_s r_s} - (-1)^l e^{+\kappa_s r_s}], \tag{41}$$

$$\tilde{c}_{\epsilon_s l}(r_s) \overset{r\to\infty}{\sim} (-1)^l \frac{1}{\sqrt{2\pi\kappa_s}} [e^{-\kappa_s r_s} + (-1)^l e^{+\kappa_s r_s}], \tag{42}$$

which are both real and normalized to $W(\tilde{s},\tilde{c})=2/\pi$. This pair will be used to define a generalized K matrix $\tilde{K}_l$ that is real for negative energies. Their relationship to the base pair is given, using Eqs. (16) and (17), by

$$\begin{pmatrix} \tilde{s} \\ \tilde{c} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} W_{g-}^c + (-1)^l W_{g+}^c & -[W_{f-}^c + (-1)^l W_{f+}^c] \\ (-1)^l [W_{g-}^c - (-1)^l W_{g+}^c] & -(-1)^l [W_{f-}^c - (-1)^l W_{f+}^c] \end{pmatrix} \begin{pmatrix} f^c \\ g^c \end{pmatrix}. \tag{43}$$

To end this section on reference functions, we point out that any transformation matrix relating any two pairs defined at two different boundaries, $r_s \to 0$ and $r_s \to \infty$, respectively, contains full information on the propagation of a wave function through the long-range potential, with Z^c being one example above the threshold and W^c being one example below the threshold. Different transformations of this type represent different views of the same physics. We also point out that due to our consistent choices of normalization, namely all reference pairs having Wronskians of $2/\pi$, the determinants of all such transformations are equal to 1. They are generally not, however, either orthogonal or unitary. The physics associated with this nonunitarity is the subject of the next section.

IV. QUANTUM REFLECTION BY AND QUANTUM TRANSMISSION AND TUNNELING THROUGH THE LONG-RANGE POTENTIAL

There are two sets of reflection and transmission amplitudes that can be defined for $-1/r^\alpha$ type of potentials with $\alpha > 2$, one corresponding to a traveling wave going inside-out, another for a traveling wave going outside-in. For a traveling wave going inside-out, the reflection amplitude, $r_l^{(io)}$, and the transmission amplitude, $t_l^{(io)}$, are defined by a solution $v_{\epsilon_s l}^{(io)}$ for a $-1/r^\alpha$ potential with boundary conditions

$$v_{\epsilon_s l}^{(io)} \overset{r_s \ll 1}{\sim} f_{\epsilon_s l}^{i+} + r_l^{(io)} f_{\epsilon_s l}^{i-}$$

$$\overset{r_s \gg 1}{\sim} t_l^{(io)} f_{\epsilon_s l}^{o+}. \tag{44}$$

But since $v_{\epsilon_s l}^{(io)}$ is itself a solution for the $-1/r^\alpha$ potential, it can be written as a linear combination of either f^{o+} and f^{o-} or f^{i+} and f^{i-}. As a result, the limit signs in Eq. (44) are equivalent to equal signs. This further means that the relationship between f^{o+} and $f^{i\pm}$ can be written in terms of the reflection and transmission amplitudes as

$$f_{\epsilon_s l}^{o+} = (1/t_l^{(io)}) f_{\epsilon_s l}^{i+} + (r_l^{(io)}/t_l^{(io)}) f_{\epsilon_s l}^{i-}. \tag{45}$$

Comparing this equation with Eq. (35), we obtain

$$t_l^{(io)} = (U_{++}^{(oi)})^{-1}$$

$$= -e^{-il\pi/2} \frac{2}{(Z_{fc}^c - Z_{gs}^c) - i(Z_{fs}^c + Z_{gc}^c)}, \tag{46}$$

$$r_l^{(io)} = U_{+-}^{(oi)}/U_{++}^{(oi)}$$

$$= -\frac{(Z^c_{fc}+Z^c_{gs})-i(Z^c_{fs}-Z^c_{gc})}{(Z^c_{fc}-Z^c_{gs})-i(Z^c_{fs}+Z^c_{gc})}. \tag{47}$$

Similarly, for a traveling wave going outside-in, the reflection and transmission amplitudes are defined by a solution $v^{(oi)}_{\epsilon_s l}$ for a $-1/r^\alpha$ potential with boundary conditions

$$v^{(oi)}_{\epsilon_s l} \overset{r_s\gg 1}{\sim} f^{o-}_{\epsilon_s l} + r^{(oi)}_l f^{o+}_{\epsilon_s l}$$

$$\overset{r_s\ll 1}{\sim} t^{(oi)}_l f^{i-}_{\epsilon_s l}. \tag{48}$$

Again, this solution is precisely $v^{(oi)}_{\epsilon_s l} = t^{(oi)}_l f^{i-}_{\epsilon_s l}$ and the limit signs are equivalent to equal signs. We have, therefore,

$$f^{i-}_{\epsilon_s l} = (r^{(oi)}_l / t^{(oi)}_l) f^{o+}_{\epsilon_s l} + (1/t^{(oi)}_l) f^{o-}_{\epsilon_s l}. \tag{49}$$

Comparing it to Eq. (36), we obtain

$$t^{(oi)}_l = (U^{(oi)}_{++})^{-1} = t^{(io)}_l,$$

$$r^{(oi)}_l = -(U^{(oi)}_{+-})^*/U^{(oi)}_{++} \tag{50}$$

$$= (-1)^l \frac{(Z^c_{fc}+Z^c_{gs})+i(Z^c_{fs}-Z^c_{gc})}{(Z^c_{fc}-Z^c_{gs})-i(Z^c_{fs}+Z^c_{gc})}. \tag{51}$$

Equations (46), (47), (50), and (51) show that we have the same transmission probability $\mathcal{T}^c_l = |t^{(io)}_l|^2 = |t^{(oi)}_l|^2$, and the same reflection probability $\mathcal{R}^c_l = |r^{(io)}_l|^2 = |r^{(oi)}_l|^2$, for waves going either inside-out or outside-in. They are given by

$$\mathcal{T}^c_l(\epsilon_s) = \frac{4}{(Z^c_{fs}+Z^c_{gc})^2 + (Z^c_{fc}-Z^c_{gs})^2}, \tag{52}$$

$$\mathcal{R}^c_l(\epsilon_s) = \frac{(Z^c_{fs}-Z^c_{gc})^2 + (Z^c_{fc}+Z^c_{gs})^2}{(Z^c_{fs}+Z^c_{gc})^2 + (Z^c_{fc}-Z^c_{gs})^2}. \tag{53}$$

From $\det(Z^c)=1$, it is easy to verify that

$$\mathcal{T}^c_l + \mathcal{R}^c_l = 1. \tag{54}$$

The transmission and reflection amplitudes can now be rewritten in terms of the reflection probability and a couple of phases,

$$t^{(io)}_l = t^{(oi)}_l = \sqrt{1-\mathcal{R}^c_l}\,\exp(-il\pi/2 - i\pi/2 + i\delta^c_l), \tag{55}$$

where the phase $\delta^c_l(\epsilon_s)$ is defined by

$$\tan\delta^c_l = \frac{Z^c_{gs}-Z^c_{fc}}{Z^c_{fs}+Z^c_{gc}} \tag{56}$$

and

$$\cos\delta^c_l = \frac{Z^c_{fs}+Z^c_{gc}}{\sqrt{(Z^c_{fs}+Z^c_{gc})^2 + (Z^c_{fc}-Z^c_{gs})^2}}. \tag{57}$$

(We need both equations to define δ^c_l to within a 2π.) The reflection amplitudes can be written as

$$r^{(oi)}_l = (-1)^l \sqrt{\mathcal{R}^c_l}\,\exp[i(\delta^c_l + \phi^c_l)], \tag{58}$$

$$r^{(io)}_l = \sqrt{\mathcal{R}^c_l}\,\exp[i(\delta^c_l - \phi^c_l)], \tag{59}$$

where we have defined phase $\phi^c_l(\epsilon_s)$ by

$$\tan\phi^c_l = \frac{Z^c_{gs}+Z^c_{fc}}{Z^c_{gc}-Z^c_{fs}} \tag{60}$$

and

$$\cos\phi^c_l = \frac{Z^c_{gc}-Z^c_{fs}}{\sqrt{(Z^c_{fs}-Z^c_{gc})^2 + (Z^c_{fc}+Z^c_{gs})^2}}. \tag{61}$$

Note that there is a phase difference between reflection amplitudes for particles going inside-out and outside-in.

Equations (52)–(61) give a complete description of the quantum reflection by and transmission and tunneling through a long-range potential of the type of $-1/r^\alpha$ with $\alpha > 2$. They also give an alternative parametrization of the QDT for $\alpha > 2$ and $\epsilon_s > 0$. Instead of the three independent elements of the Z^c matrix, we can use three alternative QDT functions δ^c_l, $\mathcal{R}^c_l$, and ϕ^c_l, in terms of which the elements of the Z^c matrix can be written as

$$Z^c_{fs} = \frac{1}{\sqrt{1-\mathcal{R}^c_l}}(\cos\delta^c_l - \sqrt{\mathcal{R}^c_l}\cos\phi^c_l), \tag{62}$$

$$Z^c_{fc} = -\frac{1}{\sqrt{1-\mathcal{R}^c_l}}(\sin\delta^c_l - \sqrt{\mathcal{R}^c_l}\sin\phi^c_l), \tag{63}$$

$$Z^c_{gs} = \frac{1}{\sqrt{1-\mathcal{R}^c_l}}(\sin\delta^c_l + \sqrt{\mathcal{R}^c_l}\sin\phi^c_l), \tag{64}$$

$$Z^c_{gc} = \frac{1}{\sqrt{1-\mathcal{R}^c_l}}(\cos\delta^c_l + \sqrt{\mathcal{R}^c_l}\cos\phi^c_l). \tag{65}$$

Each alternative has its own characteristics and utilities. The Z^c matrix comes most naturally from the mathematical solutions of Eq. (5) [8,9,14,19,21], while the reflection probability and phases have the clearest physical interpretation. Specifically, $\mathcal{R}^c_l$ is the quantum reflection probability that in some cases is directly observable [37]. δ^c_l is the long-range phase shift associated with the transmission amplitude. It will be called the long-range transmission phase shift, or the long-range phase shift for short. ϕ^c_l will be called the long-range reflection phase shift. It determines the phase differences both between the reflection and the transmission amplitudes and between the reflection amplitudes for particles going inside-out and outside-in. Similar to the Z^c matrix, the parameters δ^c_l, $\mathcal{R}^c_l$, and ϕ^c_l are all universal functions of the scaled energy ϵ_s that are uniquely determined by α.

The parametrization using δ^c_l, $\mathcal{R}^c_l$, and ϕ^c_l helps us to establish a clear relationship between quantum reflection and the structure of QDT for $\alpha > 2$. It also provides us with a quantitative measure that separates the quantum and the semiclassical regions of energies. From either Eq. (53) or from Eqs. (62)–(65), it is easily deduced that $\mathcal{R}^c_l = 0$ if and only if Z^c is orthogonal. This means the following: (a) $\mathcal{R}^c_l$ is a measure of the orthogonality of the Z^c matrix, and therefore determines the number of independent parameters required

to characterize it. (b) Since the semiclassical Z^c, as given by Eq. (B4), is orthogonal, $\mathcal{R}_l^c$ is also a measure of the deviation from the semiclassical approximation. It serves as an "order parameter" with the region of $\mathcal{R}_l^c \neq 0$ corresponding to the quantum region, and the region of $\mathcal{R}_l^c \approx 0$ corresponding to the semiclassical region. These points are conveniently summarized in the following equation, directly from Eqs. (62)–(65), which we call the semiclassical limit for Z^c:

$$Z^c \overset{\mathcal{R}_l^c \to 0}{\sim} \begin{pmatrix} \cos \delta_l^c & -\sin \delta_l^c \\ \sin \delta_l^c & \cos \delta_l^c \end{pmatrix}. \tag{66}$$

It is a much more precise version of the semiclassical limit for Z^c than using the limit of $\epsilon_s \to \infty$, which would have provided only trivial information. Through $\mathcal{R}_l^c$ we know how the semiclassical limit is reached, how accurate it is at a certain energy, and how the Z^c matrix goes from requiring three independent parameters in the quantum region of $\mathcal{R}_l^c \neq 0$ to requiring only a single parameter δ_l^c in the semiclassical region of $\mathcal{R}_l^c \approx 0$.

From Eq. (2), it is also clear that it is in this limit of $\mathcal{R}_l^c \to 0$ that Eq. (2) becomes equivalent to Eq. (1). In other words, the QDT for $\alpha > 2$ becomes structurally the same as that for $\alpha \leq 2$ only for energies at which there is no appreciable quantum reflection (the semiclassical limit). We will get back to the discussion of the physical meaning of Eq. (2) in Sec. VII. Further discussion of the structural differences between QDT for $\alpha > 2$ and $\alpha \leq 2$ can be found in Appendix C.

V. QUANTUM CONNECTION FORMULAS

For negative energies ($\epsilon_s < 0$), there is no longer any transmitted wave into the classically forbidden region. And there is no traveling wave going outside-in. There are, however, still two reflection amplitudes that can be defined, by

$$f^{o+} = C(f^{i+} + r^{(io)+} f^{i-}) \tag{67}$$

and

$$f^{o-} = C(f^{i+} + r^{(io)-} f^{i-}), \tag{68}$$

for reference functions with exponentially decreasing (f^{o+}) and exponential increasing (f^{o-}) boundary conditions at large r_s, respectively. From Eq. (37), we obtain

$$r_l^{(io)+} = \frac{W_{g-}^c - iW_{f-}^c}{W_{g-}^c + iW_{f-}^c} = \exp(i2\Phi_l^c). \tag{69}$$

It is a pure phase with $|r_l^{(io)+}|^2 = 1$, as to be expected for $\epsilon_s < 0$. Here Φ_l^c, which we call the reflection phase for f^{o+}, is defined by

$$\tan \Phi_l^c = -W_{f-}^c / W_{g-}^c \tag{70}$$

and

$$\cos \Phi_l^c = W_{g-}^c / D_l^{c+}, \tag{71}$$

in which the amplitude D_l^{c+} is defined by

$$D_l^{c+} = \sqrt{(W_{f-}^c)^2 + (W_{g-}^c)^2}. \tag{72}$$

Similarly, we have from Eq. (37)

$$r_l^{(io)-} = \frac{W_{g+}^c - iW_{f+}^c}{W_{g+}^c + iW_{f+}^c} = \exp(i2\Theta_l^c), \tag{73}$$

where Θ_l^c, the reflection phase for f^{o-}, is defined by

$$\tan \Theta_l^c = -W_{f+}^c / W_{g+}^c \tag{74}$$

and

$$\cos \Theta_l^c = W_{g+}^c / D_l^c, \tag{75}$$

in which the amplitude D_l^c is defined by

$$D_l^c = \sqrt{(W_{f+}^c)^2 + (W_{g+}^c)^2}. \tag{76}$$

In terms of the two phases Φ_l^c and Θ_l^c, and the two amplitudes D_l^{c+} and D_l^c, the W^c matrix can be rewritten as

$$W^c = \begin{pmatrix} -D_l^c \sin \Theta_l^c & -D_l^{c+} \sin \Phi_l^c \\ D_l^c \cos \Theta_l^c & D_l^{c+} \cos \Phi_l^c \end{pmatrix}. \tag{77}$$

The four parameters are not all independent. $\det(W^c) = 1$ means that they are related by

$$D_l^{c+} D_l^c \sin(\Phi_l^c - \Theta_l^c) = 1. \tag{78}$$

Equations (77) and (78) suggest an alternative description of the propagation of wave functions for $\epsilon_s < 0$. Instead of W^c, we can use three alternate functions such as Φ_l^c, D_l^c, and Θ_l^c.

We already know that the phases Φ_l^c and Θ_l^c have the interpretation of being the reflection phases for $f^{o\pm}$, respectively. Their physical meaning and that of the amplitudes D_l^{c+} and D_l^c can be further understood by rewriting the asymptotic forms of $f^{o\pm}$, using Eqs. (33), (10), and (11), in the limit of small r_s as

$$f_{\epsilon_s l}^{o+}(r_s) \overset{r_s \to 0}{\sim} (2/\pi)^{1/2} r_s^{\alpha/4} D_l^{c+} \cos(y - \pi/4 + \Phi_l^c)$$

$$\overset{r_s \to \infty}{\sim} \frac{1}{\sqrt{\pi \kappa_s}} \exp(-\kappa_s r_s), \tag{79}$$

$$f_{\epsilon_s l}^{o-}(r_s) \overset{r_s \to 0}{\sim} -(2/\pi)^{1/2} r_s^{\alpha/4} D_l^c \cos(y - \pi/4 + \Theta_l^c)$$

$$\overset{r_s \to \infty}{\sim} \frac{1}{\sqrt{\pi \kappa_s}} \exp(+\kappa_s r_s), \tag{80}$$

in which the second line of each equation is simply from the definitions of $f^{o\pm}$.

Equations (79) and (80) give what we call the quantum connection formulas. They are fully quantum results for connecting two regions, $r_s \to 0$ and $r_s \to \infty$, in which the semiclassical approximation is rigorously applicable (not an approximation). It is clear from these equations that D_l^{c+}, Φ_l^c, D_l^c, and Θ_l^c represent the amplitudes and the phases of $f^{o\pm}$ in the region of $r_s \ll 1$. The corresponding semiclassical connection formulas are Eqs. (B11) and (B12) given in Appendix B. It is clear that unlike the semiclassical connection formulas, the amplitudes D_l^{c+} and D_l^c are generally not the inverse of

TABLE I. The structure of QDT for $-1/r^\alpha$ type of potentials with $\alpha>2$. Independent QDT functions required to describe states of positive energies ($\epsilon_s>0$) and states of negative energies ($\epsilon_s<0$). There are two distinctive energy regions in both cases: a quantum region (characterized by $\mathcal{R}_l^c\neq 0$ for $\epsilon_s>0$ and by $\mathcal{Q}_l^c \neq 0$ for $\epsilon_s<0$) and a semiclassical region (characterized by $\mathcal{R}_l^c\approx 0$ for $\epsilon_s>0$ and by $\mathcal{Q}_l^c\approx 0$ for $\epsilon_s<0$).

	$\epsilon_s>0$	No. of functions	Conditions	$\epsilon_s<0$	No. of functions	Conditions
Quantum	Z^c matrix	3	None	W^c matrix	3	None
	or δ_l^c, $\mathcal{R}_l^c$, and ϕ_l^c	3	None	or Φ_l^c, D_l^c, and Θ_l^c	3	None
Semiclassical	δ_l^c	1	$\mathcal{R}_l^c\approx 0$	Φ_l^c and D_l^c	2	$\mathcal{Q}_l^c\approx 0$

each other, and the phases Φ_l^c and Θ_l^c do not always differ by $\pi/2$.

By comparing either Eqs. (77) and (78) with the semiclassical W^c as given by Eq. (B8), or by comparing Eqs. (79) and (80) with the corresponding semiclassical connection formulas, Eqs. (B11) and (B12), it is easily deduced that W^c, with generally three independent parameters, reduces to that of the semiclassical approximation with two independent parameters if and only if $\sin(\Phi_l^c-\Theta_l^c)=1$, namely, when the phases corresponding to f^{o+} and f^{o-}, respectively, differ by $\pi/2$. This criterion can be more conveniently expressed as $\mathcal{Q}_l^c=0$, where $\mathcal{Q}_l^c$ is an "order parameter" for negative energies defined by

$$\mathcal{Q}_l^c = -\frac{W_{f+}^c W_{f-}^c + W_{g+}^c W_{g-}^c}{\sqrt{[(W_{f+}^c)^2+(W_{g+}^c)^2][(W_{f-}^c)^2+(W_{g-}^c)^2]}} = -\cos(\Phi_l^c-\Theta_l^c). \tag{81}$$

In terms of $\mathcal{Q}_l^c$, the quantum and the semiclassical regions of energies below the threshold can be characterized by $\mathcal{Q}_l^c \neq 0$ and $\mathcal{Q}_l^c\approx 0$, respectively. And the semiclassical limit for W^c, in a similar sense as discussed earlier for Z^c, can be written as

$$W^c \overset{\mathcal{Q}_l^c\to 0}{\sim} \begin{pmatrix} D_l^c\cos\Phi_l^c & -(1/D_l^c)\sin\Phi_l^c \\ D_l^c\sin\Phi_l^c & (1/D_l^c)\cos\Phi_l^c \end{pmatrix}. \tag{82}$$

Table I summarizes the structure of QDT for $\alpha>2$, namely the independent functions required to describe states of positive energies $\epsilon_s>0$ and states of negative energies $\epsilon_s<0$. Some further comments related to the quantum connection formulas can be found in Appendix D.

VI. QUANTUM-DEFECT AND OTHER SHORT-RANGE PARAMETERS

With the knowledge developed in the previous sections about the long-range potential, we are now ready to construct the QDT for any real two-body interaction $V(r)$, which is necessarily different from $-C_\alpha/r^\alpha$ at short distances for $\alpha>2$.

Consider a quantum system described by the radial Schrödinger equation,

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2\mu r^2}+V(r)-\epsilon\right)u_{\epsilon l}(r)=0, \tag{83}$$

in which the potential $V(r)$ has an asymptotic behavior characterized by

$$V(r) \overset{r\to\infty}{\sim} -C_\alpha/r^\alpha. \tag{84}$$

Let r_0 to be the radius at which the potential becomes well represented by Eq. (84). For any $r\geq r_0$, the regular solution of Eq. (83), namely the solution that satisfies the boundary condition of $\lim_{r\to 0} u_{\epsilon l}\to 0$, at the origin, can always be written as a linear combination of the base pair f^c and g^c, as

$$u_{\epsilon l}(r)=A_{\epsilon l}[f_{\epsilon_s l}^c(r_s)-K^c(\epsilon,l)g_{\epsilon_s l}^c(r_s)]. \tag{85}$$

This equation defines the short-range K^c matrix [25], which can be obtained by matching the regular solution $u_{\epsilon l}$ with Eq. (85) at any $r\geq r_0$, yielding

$$K^c(\epsilon,l)=\left(\frac{f_{\epsilon_s l}^c}{g_{\epsilon_s l}^c}\right)\frac{(f_{\epsilon_s l}^{c\prime}/f_{\epsilon_s l}^c)-(u_{\epsilon l}^\prime/u_{\epsilon l})}{(g_{\epsilon_s l}^{c\prime}/g_{\epsilon_s l}^c)-(u_{\epsilon l}^\prime/u_{\epsilon l})}, \tag{86}$$

where the derivatives are with respect to r, not the scaled radius r_s.

We briefly summarize some of the key properties of K^c here, as they have been discussed elsewhere [25,27,53] (a) It is well defined for all energies and all l. (b) It is a slowly varying function of energy around the threshold. (c) For potentials ($\alpha>3$) with a well-defined s-wave scattering length $a_{l=0}$, $K^c(\epsilon=0,l=0)$ is related to the s wave scattering length by [17,27,54]

$$a_{l=0}/\beta_\alpha=\left(b^{2b}\frac{\Gamma(1-b)}{\Gamma(1+b)}\right)\frac{K^c(0,0)+\tan(\pi b/2)}{K^c(0,0)-\tan(\pi b/2)}, \tag{87}$$

where $b=1/(\alpha-2)$. (d) For atom-atom or ion-atom interactions, K^c is approximately independent of l. Some important consequences of this property have been addressed elsewhere [23,25,27,54].

Among these properties, the l-insensitivity is strictly a molecular property due to a combination of a strongly repulsive interaction, rising faster than $1/r^2$ at short distances, and large masses of atoms compared to electrons, in addition to $\alpha>2$ [25,27,53]. It is not applicable to electron-atom interactions [6,9,10,13,33–35] where the angular momentum term actually dominates the interaction near the origin. On a related mathematical note, for $V(r)$ rising faster than $1/r^2$ at

small r and $\alpha>3$, $K^c(\epsilon,l)$ is an analytic function of both ϵ and l with only simple poles. This comes from Eq. (86) by combining the properties of f^c and g^c discussed in Sec. III and applying the theorem of Poincaré [51,52] to $u_{\epsilon l}$.

In terms of K^c, the short-range phase shift, $\delta^s(\epsilon,l)$, is defined by

$$K^c(\epsilon,l) = \tan\ \delta^s(\epsilon,l), \tag{88}$$

and the quantum defect, $\mu^c(\epsilon,l)$, is defined as a parameter in a range of $0 \le \mu^c < 1$ and related to K^c by

$$K^c(\epsilon,l) = \tan[\pi\mu^c(\epsilon,l) + \pi b/2]. \tag{89}$$

This definition of a quantum defect facilitates a simple classification of molecules as discussed in Ref. [27]. Further advantages of using the quantum defect to parametrize the spectrum will be illustrated elsewhere.

The short-range S matrix, $S^c(\epsilon,l)$, is the S matrix defined in reference to f^{i+} and f^{i-}. Specifically, it is defined in the region of $r \ge r_0$ by

$$u_{\epsilon l}(r) = C[f^{i-}_{\epsilon_s l}(r_s) + S^c(\epsilon,l) f^{i+}_{\epsilon_s l}(r_s)]. \tag{90}$$

From Eq. (27), it is easy to show that

$$S^c = \frac{1+iK^c}{1-iK^c} = e^{i2\delta^s}. \tag{91}$$

The short-range parameters δ^s, μ^c, and S^c all have properties similar to those of K^c. In particular, they are all insensitive to l for atom-atom or ion-atom interactions. This explains our removal of their explicit l dependence from their respective subscripts. There is one subtlety about this l-insensitivity that is worth pointing out here. From Eq. (85), it is clear that $K^c \to +\infty$ describes the same physics as $K^c \to -\infty$, both corresponding to $u_{\epsilon l} \sim g^c$, differing only in an arbitrary overall phase factor of π. This means that a positive $K^c \gg 1$ is approximately the same as a negative K^c with $|K^c| \gg 1$. In a similar sense, a $\mu^c \sim 0$ is "close" to a $\mu^c \sim 1$, and so on.

The parameter K^{c0} is the K matrix corresponding to the reference pair f^{c0} and g^{c0}. Specifically, it is defined, in the region of $r \ge r_0$, by

$$u_{\epsilon l}(r) = C[f^{c0}_{\epsilon_s l}(r_s) - K^{c0}_l(\epsilon) g^{c0}_{\epsilon_s l}(r_s)]. \tag{92}$$

From the relationship between the f^{c0},g^{c0} pair and the base pair f^c and g^c, as given by Eq. (24), it is easy to show that K^{c0} is related to K^c by

$$K^{c0}_l(\epsilon) = \frac{K^c(\epsilon,l) - \tan(\pi\nu_0/2)}{1 + K^c(\epsilon,l)\tan(\pi\nu_0/2)} \tag{93}$$

$$= \tan[\pi\mu^c(\epsilon,l) - \pi l b]. \tag{94}$$

This parameter is closely related to the parameter $K^0_l(\epsilon)$ used in our earlier works [19,20], specifically $K^{c0}_l = -K^0_l$. It is the same as the parameter that we called $x_l(\epsilon)$ in Refs. [27,28].

The parameter $K^{c0}_l(\epsilon)$ had a disadvantage in earlier works because it depends on l explicitly through $\nu_0 = (2l+1)/(\alpha - 2)$, thus hiding the relation between the short-range parameters for different l. This is, however, no longer an issue, as knowing K^c to be approximately independent of l tells us how $K^{c0}_l(\epsilon)$ will depend on l through Eq. (93). It is still the most convenient parameter to use for near-threshold expansions [20]. It is also most convenient for describing either a bound state or a shape resonance state that is close to the threshold, since $K^{c0}_l(\epsilon=0)=0$ corresponds exactly to having a bound or a quasibound state of angular momentum l right at the threshold [23,27,28].

VII. SCATTERING STATES

For states with $\epsilon>0$, the scattering properties are determined by the asymptotic behaviors of the regular solution $u_{\epsilon l}$ in the limit of $r \to \infty$. These properties can be described using either a K matrix or an S matrix. Both formulations are addressed here as they provide different physical insights.

A. *K* matrix description

The K matrix is defined by

$$u_{\epsilon l}(r) \overset{r\to\infty}{\sim} C[s_{\epsilon_s l}(r_s) - K_l(\epsilon) c_{\epsilon_s l}(r_s)] \tag{95}$$

for positive energies. From the definitions of s and c, it is easy to see that is related to the phase shift in the standard fashion,

$$K_l = \tan\ \delta_l. \tag{96}$$

From the definitions of K_l and K^c, and the transformation between f^c, g^c and s, c, as given by Eq. (40), we obtain Eq. (2) and its representation in terms of δ^c_l, $\mathcal{R}^c_l$, and ϕ^c_l,

$$K_l = \tan\ \delta_l = (Z^c_{gc}K^c - Z^c_{fc})(Z^c_{fs} - Z^c_{gs}K^c)^{-1}$$

$$= \frac{\sin(\delta^c_l + \delta^s) + \sqrt{\mathcal{R}^c_l}\sin(\delta^s - \phi^c_l)}{\cos(\delta^c_l + \delta^s) - \sqrt{\mathcal{R}^c_l}\cos(\delta^s - \phi^c_l)}, \tag{97}$$

where the second line of the equation follows from the first by using Eqs. (62)–(65).

Equation (2) and (97) gives a complete characterization of two-body single-channel scattering by a potential $V(r) \to -C_\alpha/r^\alpha$ in terms of a set of universal functions that depends only on α, and a short-range parameter K^c that depends weakly on energy around the threshold. For atom-atom or ion-atom interactions where K^c is approximately independent of l, they also imply that the scattering of one partial wave is related to that of the other, such that, e.g., one can predict the d scattering from the s wave scattering length [23,25,29].

From Eq. (97), it is now transparent that K_l reduces to the form of Eq. (1) only in the absence of quantum reflection. It has a semiclassical limit, in the sense discussed earlier, given by

$$K_l \overset{\mathcal{R}^c_l\to 0}{\sim} \tan(\delta^c_l + \delta^s). \tag{98}$$

The characterization of the effects of the long-range potential on scattering goes from requiring three independent functions in the quantum region of $\mathcal{R}^c_l \neq 0$, such as δ^c_l, $\mathcal{R}^c_l$,

and ϕ_l^c in Eq. (97), to a single function, δ_l^c, in the semiclassical region of $\mathcal{R}_l^c \approx 0$.

Getting back again to the comparison between Eqs. (2) and (1), it should now be clear that Eq. (2) gives a more general description of the effects of the long-range interaction on two-body scattering. It is a description that is in fact applicable to *any* long-range potential. A casual examination of the definitions of the Z^c matrix and the K^c parameter immediately reveals that they are completely generic, and can be done for any potential, including the ones with $\alpha \leq 2$ and the ones with multiple length scales such as $-C_6/r^6 - C_8/r^8$. Equation (2) should thus be the form that we can take for granted. In comparison, Eq. (1) is a special case of Eq. (2) that results when the corresponding Z^c matrix becomes orthogonal. For potentials that behaves like $-1/r^\gamma$ with $\gamma > 2$ around the origin (here γ may differ from α), this orthogonality is conveniently measured by one and only one quantity, the reflection probability by the long-range potential $\mathcal{R}_l^c$. What exactly happens in the quantum regime of $\mathcal{R}_l^c \neq 0$ will become more clear in the S matrix formulation.

B. S matrix description

The S matrix is defined by

$$u_{\epsilon l}(r) \overset{r\to\infty}{\sim} C[f^{o-}_{\epsilon_s l}(r_s) - (-1)^l S_l(\epsilon) f^{o+}_{\epsilon_s l}(r_s)] \tag{99}$$

for all energies.

For positive energies, it is related to the K_l matrix and the phase shift in the standard fashion,

$$S_l = \frac{1 + iK_l}{1 - iK_l} = e^{i2\delta_l}. \tag{100}$$

From Eq. (2), S_l can be written in terms of the short-range K^c and the Z^c matrix as

$$S_l = \frac{Z^c_{fs} - Z^c_{gs}K^c - i(Z^c_{fc} - Z^c_{gc}K^c)}{Z^c_{fs} - Z^c_{gs}K^c + i(Z^c_{fc} - Z^c_{gc}K^c)}. \tag{101}$$

This equation does not offer much extra physical insight than that already contained in the K matrix formulation. More interesting is the following equation giving the S matrix in the δ_l^c, $\mathcal{R}_l^c$, and ϕ_l^c representation:

$$S_l = -\sqrt{\mathcal{R}_l^c}\exp[i(\delta_l^c + \phi_l^c)] + \frac{(1 - \mathcal{R}_l^c)\exp(i2\delta_l^c)S^c}{1 - \sqrt{\mathcal{R}_l^c}\exp[i(\delta_l^c - \phi_l^c)]S^c}. \tag{102}$$

It can be easily derived, e.g., by substituting Eqs. (62)–(65) into Eq. (101).

For conceptual understanding, we give here an alternative view of Eq. (102) that makes its underlying physics more transparent. First, note that the S matrix is closely related to the reflection amplitude by the full potential, $V(r)$, for a traveling wave going outside-in. This amplitude, $r_l^{(oi)V}$, is defined, for $\epsilon > 0$, by

$$u_{\epsilon l}(r) \overset{r\to\infty}{\sim} C[f^{o-}_{\epsilon_s l}(r_s) + r_l^{(oi)V}(\epsilon) f^{o+}_{\epsilon_s l}(r_s)], \tag{103}$$

and differs from S_l only by a phase factor, $S_l = -(-1)^l r_l^{(oi)V}$. From Eqs. (90), (45), and (49), it is straightforward to show that $r_l^{(oi)V}$ can be written in terms of the reflection and transmission amplitudes for the long-range potential and the short-range S matrix S^c as

$$r_l^{(oi)V} = r_l^{(oi)} + \frac{t_l^{(oi)} S^c t_l^{(io)}}{1 - r_l^{(io)} S^c}$$

$$= r_l^{(oi)} + t_l^{(oi)} S^c t_l^{(io)} [1 + r_l^{(io)} S^c + (r_l^{(io)} S^c)^2 + \cdots]. \tag{104}$$

Equation (104) is exactly Eq. (102) expressed in terms of reflection and transmission amplitudes, but with much more transparent physics interpretation. Keeping in mind that S^c, as defined by Eq. (90), is precisely the reflection amplitude by the short-range interactions for a particle going outside-in, we have the following physical picture. Without quantum reflection ($\mathcal{R}_l^c \to 0$), there is only a single path for scattering: the particle goes all the way into the short-range region and comes all the way back to infinity. The physics in this energy region is contained in the semiclassical limit of S_l, which follows directly from Eq. (102),

$$S_l \overset{\mathcal{R}_l^c \to 0}{\sim} \exp[i2(\delta_l^c + \delta^s)]. \tag{105}$$

It is an equation that we already understand from the K matrix formulation. With quantum reflection, the picture changes completely. The simple two-body potential scattering has now multiple paths to take, and the resulting amplitude is a coherent superposition of all the amplitudes for different paths. The first term in Eq. (104) is the amplitude for reflection by the long-range potential, completely independent of the short-range interactions. The second term is the amplitude for a path in which the particle first gets into the inner region, with amplitude $t_l^{(oi)}$, reflected back by the short-range potential, with amplitude S^c, then comes out without being reflected any further back into the short-range region, with an amplitude of $t_l^{(io)}$. The third term corresponds to a path in which the particle gets into the short-range region twice, once after being reflected back on its way out. In general, the term containing $(r_l^{(io)} S^c)^j$ corresponds to a path in which the particle is reflected back j times by the long-range potential on its way out.

Equation (102) can now be understood, quantitatively, as follows. Scattering in the quantum regime by a potential $V(r) \to -C_\alpha/r^\alpha$ with $\alpha > 2$ consists of a background due to the long-range potential only, and an interference pattern due to the particles being reflected back into the short-range region different numbers of times by the long-range interaction before they eventually emerge. All interesting energy-dependent features in the quantum region, such as shape resonances, can be understood as being the results of such interference. Similar to other conceptual understandings that emerge from the QDT [1–4], this physical picture requires no assumption about short-range interactions.

Equation (102) also makes it more transparent to model complete-absorbing short-range potentials using $S^c = 0$. This

is an effective single-channel model of a multichannel problem in which the probability for a particle to be scattered into other channels by the short-range interactions is 1. In this case, Eq. (102) gives $S_l=-\sqrt{\mathcal{R}_l^c}\exp[i(\delta_l^c+\phi_l^c)]$, independent of short-range interactions, meaning that the universal quantum reflection amplitude by the pure long-range $-1/r^\alpha$ potential becomes directly observable in such experiments [37].

C. Normalization of the continuum wave function

To understand transitions involving continuum states, such as photodissociation or photoassociation (see, e.g., Ref. [55]), we need not only the phase shifts but also the normalized wave functions. While there is always some arbitrariness in the normalization of a continuum state, one of the most useful choices is the normalization per unit energy.

An energy-normalized regular wave function, call it $F_{\epsilon l}(r)$, is normalized according to

$$\int_0^\infty F_{\epsilon' l}(r)F_{\epsilon l}(r)dr=\delta(\epsilon'-\epsilon). \tag{106}$$

It corresponds to an asymptotic form of [1–4]

$$F_{\epsilon l}(r)\overset{r_s\to\infty}{\sim}\left(\frac{2\mu}{\hbar^2\pi k}\right)^{1/2}\sin(kr-l\pi/2+\delta_l). \tag{107}$$

Comparing it with the asymptotic form of Eq. (85), it is straightforward to show that $F_{\epsilon l}(r)$ is given, in the region of $r\geq r_0$, by Eq. (85) with a normalization constant

$$A_{\epsilon l}=\left(\frac{\mu\beta_\alpha}{\hbar^2}\right)^{1/2}\frac{1}{\sqrt{(Z_{fs}^c-K^cZ_{gs}^c)^2+(Z_{fc}^c-K^cZ_{gc}^c)^2}} \tag{108}$$

$$=\left(\frac{\mu\beta_\alpha}{\hbar^2}\right)^{1/2}\frac{|\cos\delta^s|\sqrt{1-\mathcal{R}_l^c}}{\sqrt{1-2\sqrt{\mathcal{R}_l^c}\cos(\delta_l^c-\phi_l^c+2\delta^s)+\mathcal{R}_l^c}}. \tag{109}$$

VIII. STATES OF NEGATIVE ENERGIES

A. The S and the generalized K matrix for negative energy

Equation (99) defines the S matrix for all energies. For negative energies, we have from Eq. (32)

$$S_l=-(-1)^l\frac{W_{f+}^c-K^cW_{g+}^c}{W_{f-}^c-K^cW_{g-}^c} \tag{110}$$

$$=-(-1)^l(D_l^c)^2\sin(\Phi_l^c-\Theta_l^c)\frac{\sin(\Theta_l^c+\delta^s)}{\sin(\Phi_l^c+\delta^s)}, \tag{111}$$

where the second line follows from the first by using Eqs. (77) and (78). Note that S_l is real for any real $\epsilon<0$.

The generalized K matrix for $\epsilon<0$ is the K matrix corresponding to the $\tilde{s}$, $\tilde{c}$ reference pair defined in Sec. III. Specifically, it is defined by

$$u_{\epsilon l}(r)\overset{r\to\infty}{\sim}C[\tilde{s}_{\epsilon_s l}(r_s)-\tilde{K}_l(\epsilon)\tilde{c}_{\epsilon_s l}(r_s)]. \tag{112}$$

From Eq. (43), which relates the $\tilde{s}$, $\tilde{c}$ pair to f^c and g^c, we have

$$\tilde{K}_l=\frac{W_{f-}^c+(-1)^lW_{f+}^c-K^c[W_{g-}^c+(-1)^lW_{g+}^c]}{W_{f-}^c-(-1)^lW_{f+}^c-K^c[W_{g-}^c-(-1)^lW_{g+}^c]} \tag{113}$$

$$=\frac{\sin(\Phi_l^c+\delta^s)+(-1)^l(D_l^c)^2\sin(\Phi_l^c-\Theta_l^c)\sin(\Theta_l^c+\delta^s)}{\sin(\Phi_l^c+\delta^s)-(-1)^l(D_l^c)^2\sin(\Phi_l^c-\Theta_l^c)\sin(\Theta_l^c+\delta^s)}. \tag{114}$$

It is real and is related to the S matrix for negative energies by

$$\tilde{K}_l=\frac{1-S_l}{1+S_l}. \tag{115}$$

Their semiclassical limits, in the sense discussed earlier, are given by

$$S_l\overset{\mathcal{Q}_l^c\to0}{\sim}(-1)^l(D_l^c)^2\cot(\Phi_l^c+\delta^s) \tag{116}$$

and

$$\tilde{K}_l\overset{\mathcal{Q}_l^c\to0}{\sim}\frac{\tan(\Phi_l^c+\delta^s)-(-1)^l(D_l^c)^2}{\tan(\Phi_l^c+\delta^s)+(-1)^l(D_l^c)^2}. \tag{117}$$

Note that both S_l and $\tilde{K}_l$ go from requiring three QDT functions, Φ_l^c, D_l^c, and Θ_l^c, in the quantum region of $\mathcal{Q}_l^c\neq0$, to requiring two functions, Φ_l^c and D_l^c, in the semiclassical region of $\mathcal{Q}_l^c\approx0$.

The generalized K matrix and the S matrix for negative energies contain more information about the negative energy states than the bound spectrum. They are well defined for all negative energies, and are useful beyond the standard two-body problem, when the boundary condition at large r differs from that of two-body bound states, namely when it differs from $\lim_{r_s\to\infty}u_{\epsilon l}\to0$. The generalized K matrix, which is a generalization of $K_l=\tan\delta_l$ to negative energies, has found application in treating two atoms in a trap [50]. It is also useful in the studies of liquid states [56] of many-atom quantum systems, as will be illustrated elsewhere.

B. Bound spectrum

The bound spectrum is obtained by imposing the boundary condition of $\lim_{r_s\to\infty}u_{\epsilon l}\to0$ on the the regular solution $u_{\epsilon l}$ given by Eq. (85). Using the asymptotic behaviors of f^c and g^c as given by Eqs. (16) and (17), we obtain the bound spectrum as the solutions of [25]

$$\chi_l^c(\epsilon_s)=K^c(\epsilon,l), \tag{118}$$

where

$$\chi_l^c(\epsilon_s)=W_{f-}^c(\epsilon_s,l)/W_{g-}^c(\epsilon_s,l) \tag{119}$$

$$=-\tan\Phi_l^c. \tag{120}$$

It means the bound spectrum is given by the crossing points between a universal function of a scaled energy, $\chi_l^c(\epsilon_s)$, and a

slowly varying function of energy, $K^c(\epsilon,l)$, which depends on the short-range interactions. For molecular systems where K^c is approximately independent of l, Eq. (118) means that a single parameter, K^c, μ^c, or $a_{l=0}$, determines the entire rovibrational spectrum around the threshold [23,25,27].

The bound spectrum can also be formulated or understood in other ways. From Eqs. (118) and (120), it is clear that the bound spectrum can be written as the solutions of

$$\sin(\Phi_l^c + \delta^s) = 0, \tag{121}$$

which is formally the same as the corresponding formula for $\alpha \leq 2$ [1,2,4], with Φ_l^c playing the role of the β function in Refs. [1,2,4]. It can also be formulated as the solutions of

$$\Phi_l^c + \delta^s = (v+1)\pi, \tag{122}$$

where v corresponds, for molecules, to the vibrational quantum number.

Note that the fact that the bound spectrum can be written in the form of Eq. (122), in itself, has nothing to do with the applicability of the semiclassical approximation. The Φ_l^c here is the quantum reflection phase for f^{o+} as defined by Eqs. (70) and (71), which is different, in the quantum region of $\mathcal{Q}_l^c \neq 0$, from the corresponding semiclassical phase $\bar{\Phi}_l^c$ defined in Appendix B. The same formal expression for the spectrum does mean that the breakdown of the semiclassical approximation [22,43–46,48] is more transparent in the expressions for the S and the $\tilde{K}_l$, which contain more information about the negative energy states. From Eq. (110)or Eqs. (111) and (118), it is clear that the bound spectrum corresponds to the poles of the S matrix on the negative energy axis. And from Eqs. (113) and (118), it is clear that it also corresponds to the solutions of $\tilde{K}_l = -1$. Both S and $\tilde{K}_l$ have different structures for the quantum and the semiclassical regions of energies.

C. Normalization of the bound-state wave functions

To understand transitions and their rates involving bound states, we will need, in addition to bound-state energies, their corresponding normalized wave functions. Here we emphasize that the QDT determines the wave function in the region of $r \geq r_0$ completely, including their normalizations [1–4].

From the well known [1–4] and easy-to-derive equation

$$\int_0^R u_{\epsilon l}^2 dr = \left(\frac{\hbar^2}{2\mu}\right) \lim_{\epsilon' \to \epsilon} \frac{W(u_{\epsilon' l}, u_{\epsilon l})|_{r=R}}{\epsilon' - \epsilon}, \tag{123}$$

where the derivatives in the Wronskian are with respect to r, it is straightforward to show that a bound-state wave function $F_{\epsilon_b l}(r)$, normalized according to

$$\int_0^\infty [F_{\epsilon_b l}(r)]^2 dr = 1, \tag{124}$$

is given by Eq. (85) with a normalization constant

$$A_{\epsilon_b l} = \left(\frac{\pi}{2\beta_\alpha}\right)^{1/2} \left[-\frac{d\chi_l^c(\epsilon_s)}{d\epsilon_s}\bigg|_{\epsilon_{sbl}} \right]^{-1/2} \tag{125}$$

$$= \left(\frac{\pi}{2\beta_\alpha}\right)^{1/2} |\cos \Phi_l^c| \left[\frac{d\Phi_l^c(\epsilon_s)}{d\epsilon_s}\bigg|_{\epsilon_{sbl}} \right]^{-1/2}. \tag{126}$$

Here ϵ_{sbl} is a scaled bound-state energy, namely one of the solutions of Eq. (118).

IX. CONCLUSIONS

In conclusion, we have presented a general formulation of the QDT for $-1/r^\alpha$ type of potentials with $\alpha > 2$. Its structural differences from the standard theory for $\alpha \leq 2$ or from the semiclassical theory are full explained and understood through a systematic understanding of quantum reflection above the threshold, and quantum connection formulas below the threshold. The theory is given in two equivalent representations, one in terms of the Z^c and W^c matrices that connect most naturally with the mathematical solutions for the long-range potentials [8,9,14,19,21], and the other in terms of parameters—δ_l^c, $\mathcal{R}_l^c$, ϕ_l^c above the threshold and Φ_l^c, D_l^c, Θ_l^c below the threshold—that have the clearest physical interpretation.

We note that we have discussed quantum reflection by the long-range potential in a much broader context than in the recent studies of atom-surface collisions at low temperatures [37–40]. Excluding the retardation effect, these studies correspond to our special case of $l=0$. Our theory is applicable to any l, and treats reflection due to the rapid change in potential, reflection by the potential barrier, and related tunneling through the barrier all in the same consistent framework. Furthermore, these studies have only focused on the reflection of particles going outside-in. As discussed in Sec. VII, for two-body scattering in the quantum regime, it is the multiple reflections of particles in the inner region, namely the quantum reflection by the long-range potential for a particle going inside-out, that gives rise to the interesting structures in the scattering amplitudes or cross sections, including shape resonances. This reflection amplitude for a particle going inside-out differs in phase from that for a particle going outside-in. Explicit results for quantum reflection by potentials with $\alpha = 3,4,6$ will be presented elsewhere.

For long-range potentials for which we already know the solutions ($\alpha = 3,4,6$ [8,14,19,21,57]), this work considerably improves our physical understanding of the QDT associated with them [6,9–13,18,20,21,24–26]. Above the threshold, the interesting energy-dependent features in the quantum regime, including shape resonances, can now be understood rigorously as an interference pattern. Below the threshold, the breakdown of the semiclassical approximation in the quantum regime [22,43–46,48] can now be fully understood through the quantum connection formulas. Importantly, we have identified two "order parameters," $\mathcal{R}_l^c$ above the threshold and $\mathcal{Q}_l^c$ below the threshold, that clearly separate the quantum regimes, $\mathcal{R}_l^c \neq 0$ ($\mathcal{Q}_l^c \neq 0$), from the semiclassical regimes, $\mathcal{R}_l^c \approx 0$ ($\mathcal{Q}_l^c \approx 0$), with structures of the QDT being different in each of them. Computationally, these "order parameters" help to identify the energies at which one can safely make the transition from a complex full quantum calculation to a much simpler semiclassical calculation.

For all potentials with $\alpha>2$, the theory, through a rigorous connection to the semiclassical theory, gives the "high-energy" limit of all QDT parameters and functions. The question of where in energy this transition from quantum to semiclassical behavior actually occurs, both above and below the threshold, will be addressed much more completely in future publications. Here we only point out that for positive energies, this transition occurs around the barrier height, H_{sl}, since we already know classically that $\mathcal{R}_l^c=1$ below the barrier and $\mathcal{R}_l^c=0$ above the barrier. This simple picture, while far from complete, already explains why we call these parameters "order parameters." Such terminology would not have been appropriate or meaningful if $\mathcal{R}_l^c$ were to go to zero slowly and over a large range of energies. How this picture is modified quantum mechanically [35,38,39,49], and what happens for negative energies, will require in-depth studies of individual potentials, and will be presented elsewhere.

For long-range potentials with yet unknown full quantum solutions, such as $\alpha=5$, the theory provides considerable qualitative understanding and constraints that may prove to be helpful in leading to their eventual full solutions.

This paper also serves some other practical utilities. (i) It serves as a brief review of the key concepts of the QDT for $\alpha>2$ without the interference from the related mathematical complexities. (ii) It serves to clearly identify and isolate the math problems that need to be solved; to find the Z^c and the W^c for understanding two-body scattering, bound spectrum, quantum reflection, and tunneling, and transitions from quantum to semiclassical regimes; and to further find f^c and g^c for a more complete understanding including transition rates. (iii) Since the discussions presented here are completely general and applicable to any potential with $\alpha>2$, we will not need to repeat them for each individual potential. Finally, this paper serves to define a set of standardized notions that we plan to follow in our future works. The only variation, when presenting results specific to a certain long-range potential, is that we will add an extra superscript to specify the potential, e.g., the notation of $Z^{c(6)}$ will refer to the Z^c matrix for $-1/r^6$ type of potentials, as in Appendix A.

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APPENDIX A: Z^c AND W^c MATRICES FOR $-1/r^6$ TYPE OF POTENTIALS

We summarize here the Z^c and W^c matrices for $-1/r^6$ type of potentials. They follow straightforwardly from their definitions and the analytic solutions for the $-1/r^6$ potential [19],

$$Z_{fs}^{c(6)}=\frac{2^{-1/2}G_{\epsilon_s l}(\nu)\cos\,\pi(\nu-\nu_0)}{(X_{\epsilon_s l}^2+Y_{\epsilon_s l}^2)\sin\,\pi\nu}\times\{[1-(-1)^l M_{\epsilon_s l}\tan\,\pi(\nu-\nu_0)]\sin(\pi\nu/2)X_{\epsilon_s l}+[1+(-1)^l M_{\epsilon_s l}\tan\,\pi(\nu-\nu_0)]\cos(\pi\nu/2)Y_{\epsilon_s l}\},\tag{A1}$$

$$Z_{fc}^{c(6)}=\frac{2^{-1/2}G_{\epsilon_s l}(\nu)\cos\,\pi(\nu-\nu_0)}{(X_{\epsilon_s l}^2+Y_{\epsilon_s l}^2)\sin\,\pi\nu}\times\{[\tan\,\pi(\nu-\nu_0)-(-1)^l M_{\epsilon_s l}]\sin(\pi\nu/2)X_{\epsilon_s l}+[\tan\,\pi(\nu-\nu_0)+(-1)^l M_{\epsilon_s l}]\cos(\pi\nu/2)Y_{\epsilon_s l}\},\tag{A2}$$

$$Z_{gs}^{c(6)}=\frac{2^{-1/2}G_{\epsilon_s l}(\nu)\cos\,\pi(\nu-\nu_0)}{(X_{\epsilon_s l}^2+Y_{\epsilon_s l}^2)\sin\,\pi\nu}\times\{[1+(-1)^l M_{\epsilon_s l}\tan\,\pi(\nu-\nu_0)]\cos(\pi\nu/2)X_{\epsilon_s l}-[1-(-1)^l M_{\epsilon_s l}\tan\,\pi(\nu-\nu_0)]\sin(\pi\nu/2)Y_{\epsilon_s l}\},\tag{A3}$$

$$Z_{gc}^{c(6)}=\frac{2^{-1/2}G_{\epsilon_s l}(\nu)\cos\,\pi(\nu-\nu_0)}{(X_{\epsilon_s l}^2+Y_{\epsilon_s l}^2)\sin\,\pi\nu}\times\{[\tan\,\pi(\nu-\nu_0)+(-1)^l M_{\epsilon_s l}]\cos(\pi\nu/2)X_{\epsilon_s l}-[\tan\,\pi(\nu-\nu_0)-(-1)^l M_{\epsilon_s l}]\sin(\pi\nu/2)Y_{\epsilon_s l}\}.\tag{A4}$$

Here $M_{\epsilon_s l}=G_{\epsilon_s l}(-\nu)/G_{\epsilon_s l}(\nu)$, with ν, $X_{\epsilon_s l}$, $Y_{\epsilon_s l}$, and $G_{\epsilon_s l}$, all of which are functions of the scaled energy ϵ_s, being defined in Ref. [19]. An expression for Z^c, with a different notation for the elements, was given earlier in Ref. [23].

The W^c matrix for $-1/r^6$ type of potential is given by

$$W_{f+}^{c(6)}=-\frac{G_{\epsilon_s l}(\nu)\cos\,\pi\nu}{(X_{\epsilon_s l}^2+Y_{\epsilon_s l}^2)}[(1-M_{\epsilon_s l})\sin(\pi\nu/2)X_{\epsilon_s l}+(1+M_{\epsilon_s l})\cos(\pi\nu/2)Y_{\epsilon_s l}],\tag{A5}$$

$$W_{f-}^{c(6)}=\frac{G_{\epsilon_s l}(\nu)}{2(X_{\epsilon_s l}^2+Y_{\epsilon_s l}^2)\sin\,\pi\nu}[(1+M_{\epsilon_s l})\sin(\pi\nu/2)X_{\epsilon_s l}+(1-M_{\epsilon_s l})\cos(\pi\nu/2)Y_{\epsilon_s l}],\tag{A6}$$

$$W_{g+}^{c(6)}=-\frac{G_{\epsilon_s l}(\nu)\cos\,\pi\nu}{(X_{\epsilon_s l}^2+Y_{\epsilon_s l}^2)}[(1+M_{\epsilon_s l})\cos(\pi\nu/2)X_{\epsilon_s l}-(1-M_{\epsilon_s l})\sin(\pi\nu/2)Y_{\epsilon_s l}],\tag{A7}$$

$$W_{g-}^{c(6)}=\frac{G_{\epsilon_s l}(\nu)}{2(X_{\epsilon_s l}^2+Y_{\epsilon_s l}^2)\sin\,\pi\nu}[(1-M_{\epsilon_s l})\cos(\pi\nu/2)X_{\epsilon_s l}-(1+M_{\epsilon_s l})\sin(\pi\nu/2)Y_{\epsilon_s l}].\tag{A8}$$

Note that it differs by some constant factors from the earlier expression given in Ref. [50] because the definition of W^c has been modified from that of Ref. [29].

APPENDIX B: QDT FUNCTIONS IN SEMICLASSICAL APPROXIMATION

In the classically allowed region, the base pair, defined by Eqs. (10) and (11), is given in the WKB approximation (see, e.g., Ref. [41]) by

$$f^c_{\epsilon_s l}(r_s) = \frac{(2/\pi)^{1/2}}{\sqrt{k_s(r_s)}}\cos[\Phi_{\epsilon_s l}(r_s) + \pi/4], \tag{B1}$$

$$g^c_{\epsilon_s l}(r_s) = \frac{(2/\pi)^{1/2}}{\sqrt{k_s(r_s)}}\sin[\Phi_{\epsilon_s l}(r_s) + \pi/4], \tag{B2}$$

where

$$\Phi_{\epsilon_s l}(r_s) = \lim_{r_{0s}\to 0}\left(\int_{r_{0s}}^{r_s} k_s(r'_s)dr'_s - y_0\right), \tag{B3}$$

in which $y_0=[2/(\alpha-2)]r_{0s}^{-(\alpha-2)/2}$, and $k_s(r_s)$ is defined by Eq. (7).

For $\epsilon_s>0$ and greater than the barrier height, one can easily show, from the asymptotic behaviors of Eqs. (B1) and (B2), that the Z^c matrix in the semiclassical theory is an orthogonal matrix given by

$$\bar{Z}^c = \begin{pmatrix} \cos\bar{\delta}^c_l & -\sin\bar{\delta}^c_l \\ \sin\bar{\delta}^c_l & \cos\bar{\delta}^c_l \end{pmatrix}, \tag{B4}$$

where $\bar{\delta}^c_l$ is the semiclassical phase shift due to the long-range potential, given by

$$\bar{\delta}^c_l = \lim_{r_s\to\infty}[\Phi_{\epsilon_s l}(r_s) - k_s r_s + (l+1/2)\pi/2 + \pi/2]. \tag{B5}$$

We have added a bar to the semiclassical quantities with quantum counterparts to emphasize the fact that they can differ substantially in the quantum regime. The $\bar{\delta}^c_l$ in Eq. (B4) does not become a good approximation to the quantum long-range transmission phase δ^c_l, until the quantum Z^c also converges to the same form as $\bar{Z}^c$, namely not until $\mathcal{R}^c_l\to 0$.

For $\epsilon_s<0$, the wave function is still given by Eqs. (B1) and (B2) in the classically allowed region to the left of the turning point r_{ts}, defined by $k_s(r_{ts})=0$. Using the semiclassical connection formulas (see, e.g., Ref. [58]),

$$\psi_1 \overset{r\ll r_t}{\sim} \frac{C}{\sqrt{k(r)}}\sin\left(\int_r^{r_t} k(r)dr + \pi/4\right)$$
$$\overset{r\gg r_t}{\sim} \frac{C}{2\sqrt{\kappa(r)}}\exp\left(-\int_{r_t}^{r}\kappa(r)dr\right) \tag{B6}$$

and

$$\psi_2 \overset{r\ll r_t}{\sim} \frac{C}{\sqrt{k(r)}}\cos\left(\int_r^{r_t} k(r)dr + \pi/4\right)$$
$$\overset{r\gg r_t}{\sim} \frac{C}{\sqrt{\kappa(r)}}\exp\left(+\int_{r_t}^{r}\kappa(r)dr\right) \tag{B7}$$

to propagate the wave functions to infinity, we obtain

$$\bar{W}^c = \begin{pmatrix} \bar{D}_l\cos\bar{\Phi}^c_l & -(1/\bar{D}_l)\sin\bar{\Phi}^c_l \\ \bar{D}_l\sin\bar{\Phi}^c_l & (1/\bar{D}_l)\cos\bar{\Phi}^c_l \end{pmatrix}, \tag{B8}$$

where

$$\bar{\Phi}^c_l = \Phi_{\epsilon_s l}(r_{ts}), \tag{B9}$$

and

$$\bar{D}_l(\epsilon_s) = \frac{1}{\sqrt{2}}\lim_{r_s\to\infty}\exp\left[\kappa_s r_s - \int_{r_{ts}}^{r_s}\kappa_s(r'_s)dr'_s\right]. \tag{B10}$$

Again, the semiclassical quantities $\bar{\Phi}^c_l$ and $\bar{D}_l$ do not become good approximations to their quantum counterparts until the quantum W^c converges to the same form as $\bar{W}^c$, namely not until $\mathcal{Q}^c_l\to 0$.

Using Eqs. (B6) and (B7) to connect regions $r_s\to 0$ and $r_s\to\infty$ in which the semiclassical theory is rigorously applicable, we have the semiclassical connection formulas

$$f^{o+}_{\epsilon_s l}(r_s) \overset{r_s\to 0}{\sim} (2/\pi)^{1/2} r_s^{\alpha/4}(1/\bar{D}^c_l)\cos(y - \pi/4 + \bar{\Phi}^c_l)$$
$$\overset{r_s\to\infty}{\sim} \frac{1}{\sqrt{\pi\kappa_s}}\exp(-\kappa_s r_s), \tag{B11}$$

$$f^{o-}_{\epsilon_s l}(r_s) \overset{r_s\to 0}{\sim} -(2/\pi)^{1/2} r_s^{\alpha/4}\bar{D}^c_l\sin(y - \pi/4 + \bar{\Phi}^c_l)$$
$$\overset{r_s\to\infty}{\sim} \frac{1}{\sqrt{\pi\kappa_s}}\exp(+\kappa_s r_s), \tag{B12}$$

that should be compared to the fully quantum results of Eqs. (79) and (80). We note that the semiclassical formulation here is very similar to that given by Greene *et al.* [2,4]. The slight differences are related to boundary conditions near the origin.

APPENDIX C: FURTHER COMMENTS ON THE STRUCTURE OF QDT FOR $\epsilon>0$

We discuss here some more subtle points as related to the structure of QDT for $\epsilon>0$. In the Introduction, we stated that Eq. (2) cannot generally be written in the form of Eq. (1). To be more precise, what we meant was that this cannot be done without altering the characteristics of $\delta^{(s)}_l$ for being nearly energy-independent. We show here that if we relax this criterion, namely letting $\delta^{(s)}_l$ be energy-dependent as needed, we can indeed recast the QDT for $\alpha>2$, as presented in this paper, to be in the same form as QDT for $\alpha\le 2$ [1–4]. We also discuss how the structural differences between $\alpha>2$ and $\alpha\le 2$ are reflected in such a formulation [9,18].

Define two amplitues B and B^g and two phase shifts δ^f_l and δ^g_l by

$$B = [(Z^c_{fs})^2 + (Z^c_{fc})^2]^{-1}, \tag{C1}$$

$$\tan\delta^f_l = -Z^c_{fc}/Z^c_{fs}, \tag{C2}$$

$$\cos\ \delta_l^f = B^{1/2} Z_{fs}^c, \tag{C3}$$

and

$$B^g = [(Z_{gs}^c)^2 + (Z_{gc}^c)^2]^{-1}, \tag{C4}$$

$$\tan\ \delta_l^g = -Z_{gc}^c / Z_{gs}^c, \tag{C5}$$

$$\cos\ \delta_l^g = (B^g)^{1/2} Z_{gs}^c. \tag{C6}$$

Not all four parameters are independent, as $\det(Z^c)=1$ leads to the constraint

$$(BB^g)^{-1/2} \sin(\delta_l^f - \delta_l^g) = 1. \tag{C7}$$

Further define a pair of reference functions f and g by

$$f_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} \left(\frac{2}{\pi k_s}\right)^{1/2} \sin(k_s r_s - l\pi/2 + \delta_l^f), \tag{C8}$$

$$g_{\epsilon_s l}(r_s) \overset{r_s\to\infty}{\sim} -\left(\frac{2}{\pi k_s}\right)^{1/2} \cos(k_s r_s - l\pi/2 + \delta_l^f). \tag{C9}$$

It is easy to show that f and g are related to f^c and g^c in the standard QDT fashion, with f^c and g^c playing the role of f^o and g^o of Refs. [1,2,4],

$$\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} B^{1/2} & 0 \\ B^{-1/2}\mathcal{G} & B^{-1/2} \end{pmatrix} \begin{pmatrix} f^c \\ g^c \end{pmatrix}, \tag{C10}$$

where

$$\mathcal{G} = -B\ \cot(\delta_l^f - \delta_l^g). \tag{C11}$$

Now if we define a phase shift $\delta_l^{(s)}$ using f and g as reference functions, namely by

$$u_{\epsilon l}(r) = C[f_{\epsilon_s l}(r_s) - \tan\ \delta_l^{(s)} g_{\epsilon_s l}(r_s)] \tag{C12}$$

for $r \geq r_0$, we can write

$$K_l = \tan\ \delta_l = \tan(\delta_l^f + \delta_l^{(s)}), \tag{C13}$$

where

$$\tan\ \delta_l^{(s)} = \frac{BK^c}{1 + \mathcal{G}K^c} \tag{C14}$$

with K^c playing the role of $\tan\ \delta_l^{(so)}$, or equivalently with our $\mathcal{S}^s = \tan^{-1}(K^c)$ playing the role of $\delta_l^{(so)}$ of Refs. [1,2,4].

In this formulation, which is formally the same for $\alpha > 2$ and $\alpha \leq 2$, the structural differences between $\alpha > 2$ and $\alpha \leq 2$ are reflected in the fact that whereas B and $\mathcal{G}$, and therefore $\delta_l^{(s)}$, are slowly varying functions of energy for $\alpha \leq 2$ [1–5], they have rapid energy dependence through Z^c in the quantum region of $\mathcal{R}_l^c \neq 0$ for $\alpha > 2$. This energy dependence means that, just like the other two formulations presented in the main text, we need three independent QDT functions, B, $\mathcal{G}$, and δ_l^f [9,18], to fully characterize the quantum region for $\alpha > 2$. In the semiclassical region of $\mathcal{R}_l^c \to 0$, where one can easily show that $\delta_l^f \to \delta_l^c$, $B \to 1$, $\mathcal{G} \to 0$, and $\delta_l^{(s)} \to \mathcal{S}^s$, the number of independent functions reduces to one, again just like in the other two formulations. We also note that it has long been recognized by Watanabe and Greene [9] that the rapid variation of B and $\mathcal{G}$ at small energies is due to "the penetration of the effective centrifugal barrier," a physical picture that is fully consistent with our interpretation in terms of quantum reflection and transmission.

APPENDIX D: SEMICLASSICAL-QUANTUM HYBRID THEORY

The quantum-connection formulas of Sec. V would seem to suggest an improved semiclassical theory based on it. It is indeed possible, but would be somewhat missing the point, which is that if we already know the parameters that give the quantum connection formulas, semiclassical theory is no long necessary, at least not in the region of the long-range potential.

A more useful approach is to use the semiclassical theory to obtain the short-range parameters such as K^c or S^c, namely use it inside r_0, where its applicability is often well justified especially in atom-atom or ion-atom interactions (simply because the atoms are moving much faster in the short-range region). All other aspects of the theory are kept the same as those in Secs. VII and VIII, namely the propagation of the wave function from r_0 to infinity is done fully quantum mechanically. This semiclassical-quantum hybrid approach, which has been taken, for example, by Gribakin and Flambaum in their study of ultracold atomic collisions [17,47], is useful over a much wider range of energies, and especially in a multichannel formulation [29] to study inelastic processes and other two-body reactions.

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