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Canonical quantum potential scattering theory*

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Abstract

A new formulation of potential scattering in quantum mechanics is developed using a close structural analogy between partial waves and the classical dynamics of many non-interacting fields. Using a canonical formalism we find nonlinear first-order differential equations for the low-energy scattering parameters such as scattering length and effective range. They significantly simplify typical calculations, as we illustrate for atom–atom and neutron–nucleus scattering systems. A generalization to charged particle scattering is also possible.

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1. Introduction

Low-energy scattering parameters such as the scattering length and the effective range are very important physical quantities that are used to describe a variety of systems. Among these are nuclear reactions of relevance to nucleosynthesis [1] and cold dilute atomic gases [2]. To find the low-energy scattering behaviour for a given potential, the generic approach is to solve the stationary Schrödinger equation for a range of scattering momenta and to extract the scattering phase shifts [3]. In contrast, the formalism we will present allows the computation of the scattering length and effective range directly from the potential.

To reformulate quantum scattering theory, we use methods from classical mechanics. A ‘Hamiltonian’ function expressed in terms of the coefficients of the Riccati–Bessel and Riccati–Neumann function expansion of the solution of the Schrödinger equation was found amenable to formal canonical manipulations. This Hamiltonian, of a quadratic form, can be rendered constant with an appropriate canonical transformation. From this transformation we obtain a first-order, nonlinear differential equation for the scattering problem that generalizes Calogero’s equation [4]. We demonstrate how this equation can be used to solve the scattering problem for low momenta and several partial waves for cases involving long-range

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Van der Waals-type interaction only and those involving short-range nuclear interaction only. A modified effective range theory can also be formulated for Coulomb plus short-range potentials as shown in [5], and its Calogero version is described briefly in appendix B. In the same appendix, we also briefly discuss the inherent difficulties encountered in deriving such an expansion for the Coulomb plus long-range polarization interactions, as clearly shown in [6–8].

The examples that we consider in detail in this paper range from neutron–nucleus scattering to atom–atom scattering. In the latter, the basic input into the atom–atom effective interaction is the scattering length a , defined as the scattering amplitude evaluated at zero energy $a = -f(E = 0)$, where f is determined from the $l = 0$ phase shift, $\delta_0(k)$.

The effective range expansion for $D_l(k) = \frac{\tan(\delta_l(k))}{k^{2l+1}}$ is [5],

$$\frac{1}{D_l(k)} = -\frac{1}{a_l} + \frac{1}{2}r_l k^2 - P_l r_l^3 k^4. \quad (1)$$

Our formalism allows the calculation of a_l , r_l and P_l directly from the potential, using first-order, nonlinear, differential equations, and may allow the development of new approximation schemes for the calculation of these low-energy parameters in cases where the usual procedure of solving the second-order equation (the Schrödinger equation) may be cumbersome.

This paper is organized as follows. In section 2 we present our canonical formulation of potential scattering. In section 3 we derive the Calogero-type equation for the scattering length function and obtain first-order nonlinear differential equations for the scattering length, effective range and shape parameter. In section 4, we apply the theory to the calculation of the low-energy parameters of typical atomic scattering systems. One further application to typical short-range potential nuclear scattering is presented in section 5. Finally, in section 6 several concluding remarks are made. Appendices contain the essentials of potential scattering and generalizations of our work to charged particle scattering.

2. Canonical formulation

In quantum scattering from a central potential $V(r) = \frac{\hbar^2}{2m}U(r)$, one has to solve the radial Schrödinger equation [9, 10]

$$\left[-\frac{d^2}{dr^2} + U(r) + \frac{l(l+1)}{r^2} \right] \phi_l(k, r) = k^2 \phi_l(k, r), \quad (2)$$

where l is the angular momentum quantum number, and k is the scattering momentum. It is known that the solution can be parametrized as

$$\phi_l(k, r) = u_l(kr)q_l(k, r) + v_l(kr)p_l(k, r), \quad (3)$$

where $u_l(kr)$ and $v_l(kr)$ are the Riccati–Bessel and Riccati–Neumann functions.

Following [11, 12], we construct a classical ‘Hamiltonian’ function,

$$H(q, p) = \frac{U(r)}{2k} (u_l q_l + v_l p_l)^2. \quad (4)$$

Through a straightforward computation of $\frac{dq_l}{dr}$ and $\frac{dp_l}{dr}$ from equation (2) and equations (A.5) and (A.8)–(A.10) in the appendix, we find

$$\frac{dq_l}{dr} = \frac{\partial H}{\partial p_l}, \quad (5)$$

$$\frac{dp_l}{dr} = -\frac{\partial H}{\partial q_l}. \quad (6)$$

It is therefore evident that we may regard q_l and p_l as the coordinate and conjugate momentum respectively, with r acting as the ‘time’ variable in a ‘classical’ dynamics governed by the Hamiltonian $H(q, p)$ above [13]. It should be realized that in this fashion we treat each partial wave independently as there is no coupling between waves for different l due to the spherical symmetry of $V(r)$. Thus the scattering problem is reduced to a many (strictly speaking infinite) non-interacting classical fields problem.

Any function $F_l(q, p; r)$ of q, p and r will evolve in ‘time’ r as

$$\frac{dF_l}{dr} = [F_l, H] + \frac{\partial F_l}{\partial r}, \quad (7)$$

where $[F_l, H]$ is the Poisson bracket.

In order to identify useful functions for the scattering problem, such as the phase shift, we perform a canonical transformation to a new coordinate Q_l and a new momentum P_l , using the following generating function:

$$F_2(q_l, P_l, r) = \frac{1}{2} A_l(r) q_l^2 + B_l(r) q_l P_l, \quad (8)$$

where the functions $A_l(r)$ and $B_l(r)$ are arbitrary to be determined by imposing a condition on the new dynamics, and

$$Q_l = \frac{\partial F_2}{\partial P_l} = q_l B_l(r), \quad (9)$$

and

$$p_l = \frac{\partial F_2}{\partial q_l} = A_l(r) q_l + B_l(r) P_l. \quad (10)$$

The new Hamiltonian function $K(Q_l, P_l; r)$ is

$$K(Q_l, P_l; r) = H(q_l, p_l; r) + \frac{\partial F_2(q_l, P_l; r)}{\partial r}. \quad (11)$$

It is now a simple matter to obtain the explicit form of the new Hamiltonian, K , namely

$$K(Q_l, P_l; r) = \frac{Q_l^2}{2B_l^2} \left[\frac{U(r)}{k} (u_l + v_l A_l)^2 + \frac{dA_l}{dr} \right] + \frac{Q_l P_l}{B_l} \left[\frac{U(r)}{k} v_l (u_l + v_l A_l) B_l + \frac{dB_l}{dr} \right] + \frac{U(r)}{2k} v_l^2 B_l^2 P_l^2. \quad (12)$$

The goal is now to render the new coordinate Q_l cyclic. To this end, we impose the condition that the functions $A_l(r)$ and $B_l(r)$ satisfy the first-order, non-linear differential equations

$$\frac{dA_l(r)}{dr} + \frac{U(r)}{k} (u_l(r) + v_l(r) A_l(r))^2 = 0, \quad (13)$$

and

$$\frac{dB_l(r)}{dr} + \frac{U(r)}{k} (u_l(r) + v_l(r) A_l(r)) B_l(r) = 0. \quad (14)$$

To solve these, we need to specify a boundary condition. We choose the values of the functions $A_l(0) = 0$ and $B_l(0) = 1$, which guarantee that the new coordinate Q_l and momentum P_l have the same limiting values at $r = 0$ as the original ones, q_l and p_l , namely $Q_l(r) \rightarrow 1$ and $P_l(r) \rightarrow 0$ as $r \rightarrow 0$.

With this choice of the coefficients $A_l(r)$ and $B_l(r)$, the new Hamiltonian function $K(Q_l, P_l; r)$ is

$$K(Q_l, P_l; r) = \frac{U(r)}{2k} v_l^2(r) B_l^2(r) P_l^2, \quad (15)$$

and the new equations of motion are

$$\frac{dP_l}{dr} = -\frac{\partial K}{\partial Q_l} = 0 \quad (16)$$

and

$$\frac{dQ_l}{dr} = \frac{\partial K}{\partial P_l} = \frac{U(r)}{2k} v_l^2(r) B_l^2 P_l. \quad (17)$$

We choose the solutions, $P_l(r) = 0$ and $Q_l(r) = 1$, which are consistent with the new equations of motion and the boundary conditions. With this choice, we have the solution of the original problem:

$$q_l(r) = \frac{1}{B_l(r)} \quad (18)$$

and

$$p_l(r) = \frac{A_l(r)}{B_l(r)}. \quad (19)$$

By elimination of $B_l(r)$ from the above equations, we obtain for the function $A_l(r)$ the following

$$A_l(r) = \frac{p_l(r)}{q_l(r)}, \quad (20)$$

which can be identified as the phase shift function $\tan \delta_l(r)$, introduced by Calogero [4].

For charged particle scattering, the free solutions $u_l(kr)$, $v_l(kr)$ are replaced by the scaled Coulomb wavefunctions, defined in appendix B. The equation for the tangent function $A_l(r)$ is given by a similar equation as 13, with the replacement of $u_l(kr)$ by the regular scaled Coulomb wavefunction, $\mathcal{F}_l(kr)$ and $v_l(kr)$ by the irregular scaled Coulomb wavefunction, $\mathcal{G}_l(kr)$. A detailed discussion of the charged-particle Calogero equation of the scattering length function is beyond the scope of this paper, but a brief preview is given in appendix B.

3. Scattering length function

It is convenient to introduce the scattering length function $a(k, r)$ defined as the function

$$a_l(k, r) = -\frac{A_l(r)}{k^{(2l+1)}}, \quad (21)$$

which satisfies the Calogero-type equation,

$$\frac{da_l(k, r)}{dr} - \frac{U(r)}{k^{2l+2}} (u_l(kr) - k^{(2l+1)} v_l(kr) a_l(k, r))^2 = 0. \quad (22)$$

Note that $a_l(k; \infty)$ has the dimension of L^{2l+1} .

The above equation has to be solved with the boundary condition $a_l(k, 0) = 0$. The scattering length itself is, by definition, $a_l(0, \infty)$. For $l = 0$ the equation becomes

$$\frac{da(k, r)}{dr} - \frac{U(r)}{k^2} (\sin(kr) - k \cos(kr) a(k, r))^2 = 0. \quad (23)$$

Further, specifying $k = 0$ we have

$$\frac{da(0, r)}{dr} - U(r)[r - a(0, r)]^2 = 0. \quad (24)$$

A final special case of interest is $k = 0$ and integer l . Then the asymptotic behaviour of the Bessel functions (see equations (A.19)–(A.20)) gives

$$\frac{da_l(0, r)}{dr} - U(r) \left[\frac{r^{l+1}}{(2l+1)!!} - \frac{(2l-1)!!}{r^l} a_l(0, r) \right]^2 = 0. \quad (25)$$

Equations (22) and (25) are already sufficient to extract the low-energy scattering behaviour that defines equation (1) as we shall demonstrate in the following section. However, they can also be used to obtain equations that determine the parameters of the effective range expansion directly. This can be done by expanding equation (22) in k , equating coefficients and using the identification $D_l(k) \rightarrow -a_l(k, r)$. The resulting Calogero equations for $r_0(r)$ and $p_0(r) = P_0(k, r)r_0(k, r)^3$ are

$$\frac{dr_0(r)}{dr} + 2rU(r)r_0(r) \left(\frac{r}{a_0(r)} - 1 \right) + 2r^2U(r) \left[\frac{r}{a_0(r)} - 1 \right] \left[\frac{r}{3a_0(r)} - 1 \right] = 0, \quad (26)$$

$$\frac{dp_0(r)}{dr} + 2rU(r) \left[\frac{r}{a(r)} - 1 \right] p_0(r) + F(r) = 0, \quad (27)$$

where the function $F(r)$ is given by

$$F(r) = \frac{r^2U(r)}{12}(2r - r_0(r))(2r - 3r_0(r)) + \frac{r^2U(r)}{45a_0^2(r)}[2r^4 + 3a_0(r)r^2(5r_0(r) - 4r)]. \quad (28)$$

The above two differential equations can be integrated once the $l = 0$ scattering length function, $a_0(r)$ is known. Numerically, equations (24)–(27) could be solved as a coupled system. Note that $r_0(r = 0) = 0$ and $p_0(r = 0) = 0$ owing to the boundary condition obeyed by the scattering length function $a_l(k, r = 0) = 0$.

The scattering length equation for any partial wave can be written down, with the aid of equation (22) and equations (A.19)–(A.20) of the appendix:

$$\frac{da_l(0, r)}{dr} - U(r) \left[\frac{r^{l+1}}{(2l+1)!!} - \frac{(2l-1)!!}{r^l} a_l(0, r) \right]^2 = 0. \quad (29)$$

The corresponding $l \neq 0$ version of the Calogero equations for the effective range function $r_l(r)$ and shape parameter function $p_l(r)$ can be easily worked out using the small k form of the Riccati–Bessel and Riccati–Neumann functions, given in appendix A.

Before we turn to the application of our formalism to physical systems, we specify the types of the potential $V(r)$ which allow using the effective range expansion and, consequently, the above Calogero-type equations for low-energy scattering parameters. For low-energy scattering of composite systems such as atoms or nuclei, the most general form of the interaction potential can be written as

$$V(r) = V^l(r) + V^s(r). \quad (30)$$

Here $V^l(r)$ is the long-range component, containing the $1/r$ Coulomb potential, $V_C(r)$, for charged systems, and long-range polarization components, $V_P(r)$, for example describing Van der Waals forces. Both the Coulomb and the adiabatic dipole polarization potentials arise from the one and multi-photon exchange. On the other hand $V^s(r)$ is the short-range interaction arising from the meson exchange, usually operative in nuclear scattering. The theory of effective range expansion is well founded for potentials of the types $V(r) = V_P(r)$ (atom–atom scattering), $V(r) = V^s(r)$ (neutron–nucleus scattering). A Coulomb-modified effective range expansion is also well founded [5] for potentials of the type $V(r) = V_C + V^s(r)$ (proton–nucleus and nucleus–nucleus scattering). In the scattering of a charged particle from a dipole–polarizable charged target particle (atomic ion–diatomic molecular ion, very low-energy proton–deuteron), the potential is of the long-range type only, $V(r) = V_C(r) + V_P(r)$. In this latter case, the Coulomb-modified effective range expansion fails [6–8]. However, one can still define an s-wave scattering length, albeit modified, as shown by [6, 7]. In the applications below, we restrict ourselves to the cases involving atom–atom scattering, $V(r) = V_P(r)$, and to neutron–nucleus scattering, $V(r) = V^s(r)$. The Coulomb-modified theory is briefly described in appendix B.

4. Cold atom scattering

To show how our formalism simplifies typical calculations, we now use it to determine low-energy scattering parameters for some exemplary potentials and compare our results with the literature. We shall mostly consider scattering of Cs atoms interacting with the potential [14]

$$V(r) = \frac{1}{2}\beta r^\lambda e^{-\eta r} - \left(\frac{C_6}{r^6} + \frac{C_8}{r^8} + \frac{C_{10}}{r^{10}} \right) f_c(r), \quad (31)$$

$$f_c(r) = \theta(r - r_c) + \theta(r_c - r) e^{-(r_c/r-1)^2}, \quad (32)$$

where in atomic units $\beta = 1.6 \times 10^{-3}$, $\lambda = 5.53$, $\eta = 1.072$, $C_6 = 7020$, $C_8 = 1.1 \times 10^6$, $C_{10} = 1.7 \times 10^8$, $r_c = 23.1654$, and the reduced mass of a cesium pair is $m = 1.211 \times 10^5$.

4.1. S-wave scattering length

The s-wave scattering length can be determined according to the Calogero equation (24). It has been recently used to assess corrections to calculations that rely on using the usual Schrödinger equation with long-range interactions [15]. Here, we first summarize their calculations and then extend them to other partial waves and to determining the effective range and shape parameters.

Integrating this equation is numerically non-trivial, owing to poles in $a(0, r)$ that arise from bound states in the potential. This problem can be overcome by using a symplectic integrator or a variable transformation that maps the spatial domain and the range of function values onto a compact interval [15]. For the latter one defines $\tan[\theta(r)] = a(0, r)$ and $r = \tan(\phi)$, and then solves a nonlinear equation for $\theta(\phi)$. Since equation (24) is singular at $r = 0$, the initial condition is $a(\epsilon) = 0$, with ϵ chosen sufficiently small. The determination of the Cs–Cs scattering length in this manner has been done in [15], which also shows $a(0, r)$ as a function of r to visualize the above-mentioned pole structure. The scattering length following from this potential, $a_s = 68.21$ is reproduced precisely by equation (24).

4.2. S-wave effective range expansion

Our formalism allows us to use the transformation of the preceding section to determine quantities beyond the scattering length. For the effective range, we present two methods: the direct integration of equation (26) and the integration of equation (23) for a range of k and subsequent fitting of equation (1).

4.2.1. Effective range equation. We use the substitutions $\tan[\theta_1(r)] = a(0, r)$, $\tan[\theta_2(r)] = r_0(r)$ and $r = \tan(\phi)$ in equations (24)–(26). The resulting system of two coupled equations is

$$\begin{aligned} \frac{d\theta_1(\phi)}{d\phi} - \sec^4[\phi] \sin^2[\theta_1(\phi) - \phi] U[\tan(\phi)] &= 0, \\ \frac{d\theta_2(\phi)}{d\phi} - \sec^2[\phi] \cos^2[\theta_2(\phi)] U[\tan(\phi)] &\left[2 \tan[\theta_2(\phi)] \tan(\phi) \left(1 - \frac{\tan(\phi)}{\tan[\theta_1(\phi)]} \right) \right. \\ &\left. - 2 \tan(\phi)^2 + \frac{8}{3} \frac{\tan(\phi)^3}{\tan[\theta_1(\phi)]} - \frac{2}{3} \frac{\tan(\phi)^4}{\tan[\theta_1(\phi)]^2} \right] = 0. \end{aligned} \quad (33)$$

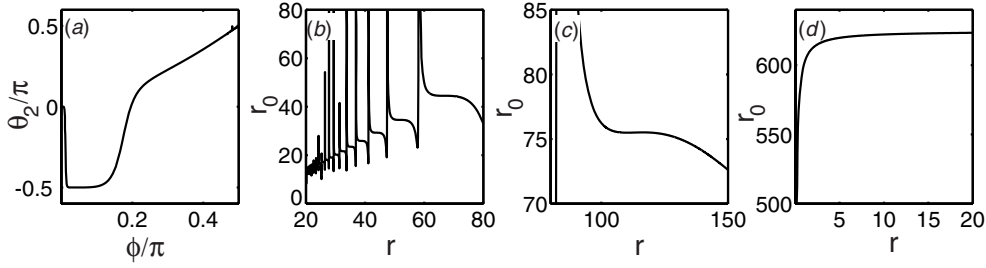


Figure 1. (a) Function $\theta_2(\phi)$ obtained from equation (33), (b)–(d) Reconstructed $r_0(r)$ for different ranges of r . The pole structure in (b) arises from bound states in the potential. The asymptotic value reached in (d) gives the physical effective range $r_0 = 623.361$.

Again we use the initial conditions $a(0, \epsilon_r) = \epsilon_a$ and $r_0(\epsilon_r) = 0$, with ϵ_a, ϵ_r small, to avoid an initial singularity. The solution is shown in figure 1; similar plots showing the scattering length can be found in [15].

4.2.2. Low k expansion. Alternatively, in equation (23) we define $\tan[\theta(k, r)] = a(k, r)$ and $r = \tan(\phi)$. This yields

$$\frac{d\theta(k, \phi)}{d\phi} - \sec^2[\phi] \cos^2[\theta(k, \phi)] \frac{V[\tan(\phi)]}{E_k} (\sin[k \tan(\phi)] - k \cos[k \tan(\phi)] \tan[\theta(k, \phi)])^2 = 0. \tag{34}$$

We now solve equation (34) for several values of k ; see figure 2. Using the effective range expansion as in equation (1) we can then extract the low-energy scattering parameters from a fit as shown. The values for a_s and r_s agree roughly those of [14] (which are $a_s = 68.22$ and $r_s = 624.55$). For the fit we varied the range of values of k under consideration until the smallest errors were reported by the fitting routine. The directly calculated effective range agrees better with [14] than that obtained from the fit. However, the fitting procedure is able to give also an indication of the shape parameter, whereas the direct determination of it, using equation (27), was plagued by numerical instabilities.

4.3. Higher partial waves

The scattering lengths for higher partial waves (p, d, f, . . .) can, in principle, be obtained from the simple equation (25). For the potential given at the beginning of this section we find $a_p = -4.38 \times 10^5 a_0^3$. Higher partial waves for the atom–atom potential cannot be treated with our method, since the centrifugal terms in equation (25) combine with the long-range tail of the potential to produce a constant slope of the scattering length function. This shortcoming is absent in the case of short-range interaction, such as that encountered in neutron–nucleus scattering, as we discuss in the following section. As additional check of our theory we reproduced the s-wave and p-wave scattering length for ^3He and ^4He given in [16], which relate to the HFDHE2 potential of [17]. This comparison is shown in table 1.

5. Nuclear scattering

For potentials that drop off faster than any polynomial at large r all the partial waves can be obtained. To demonstrate this, we apply our method to calculate the low-energy scattering

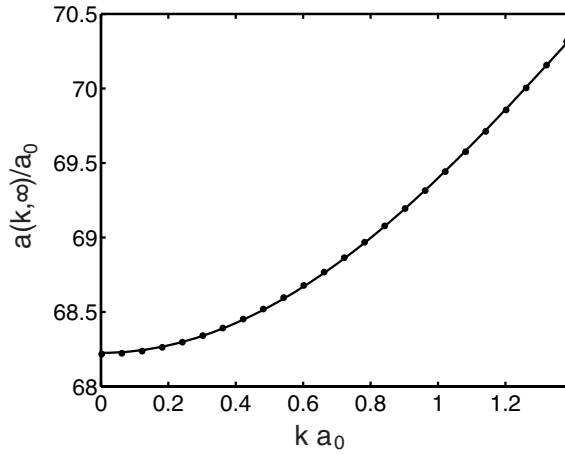


Figure 2. Asymptotic s-wave scattering length function (●) for several values of wave number k . The solid line is a least-squares fit of the function $D_0(k)$ (see equation (1)), from which we can extract the scattering length $a_s = 68.23 \pm 0.01a_0$, the effective range $r_s = 541.69 \pm 6a_0$ and the shape parameter $P_s = 0.144 \pm 0.006$. The uncertainties reflect 95% confidence bounds of the fit.

Table 1. S-wave and p-wave scattering length for the two helium isotopes.

Parameter	Present study	[16]
$^3\text{He } a_s$	-7.03\AA	-6.97\AA
$^3\text{He } a_p$	-26.15\AA^3	-26.09\AA^3
$^4\text{He } a_s$	97.21\AA	125.08\AA
$^4\text{He } a_p$	-42.67\AA^3	-42.12\AA^3

parameters for the $n + {}^{12}\text{C}$ system, where the interaction is short range and contains a spin-orbit part [18]. In the latter case, owing to the spin s of the neutron, one must specify the total angular momentum, $j = l + s$, which can take either one of two values $j = l + 1/2$ or $j = l - 1/2$. The scattering length and the other low-energy parameters acquire two labels jl . The interaction itself is split into two:

$$V(r) = V_0(r) + V_{so}(r)l \cdot s. \quad (35)$$

For $j = l + 1/2$, one has

$$V_{j=l+1/2}(r) = V_0(r) + \frac{l}{2}V_{so}(r) \quad (36)$$

and for $j = l - 1/2$, one has

$$V_{j=l-1/2}(r) = V_0(r) - \frac{l+1}{2}V_{so}(r). \quad (37)$$

In the above equations the spherical potential is denoted by $V_0(r)$ and is invariably taken to have a Fermi-type dependence on r , the so-called the Woods–Saxon shape

$$V_0(r) = -\frac{V_0}{1 + \exp\left(\frac{r-R}{d}\right)}, \quad (38)$$

while the spin–orbit potential $V_{so}(r)$ is given by

$$V_{so}(r) = \frac{5.5}{1 + \exp\left(\frac{r-R}{d}\right)}. \quad (39)$$

Table 2. Scattering length (in fm^{2l+1}) and effective range (in fm^{-2l+1}) for different angular momentum channels of a $n + {}^{12}\text{C}$ collision [18]. Underlines indicate the results from the present study. The well depth of the channels, V_0 (in MeV), is also shown.

l, s	V_0	$a_{l,s}$	$a_{l,s}, [18]$	$r_{l,s}$	$r_{l,s}, [18]$	$p_{l,s}$
s, 1/2	57.6	6.51	6.43	3.58	3.56	-0.055
p, 3/2	45.1	9.16	8.85	-1.68	-1.71	0.038
p, 1/2	45.1	23.21	22.75	-1.15	-1.16	0.26
d, 5/2	56.15	179.6	159.9	-0.32	-0.32	-28.65
d, 3/2	56.15	-56.1	-57.2	-0.061	-0.065	-2864

As in section 4.2, we extract the scattering length and effective range from a fit to the low momentum behaviour of $a_{l,s}(k, \infty)$. A comparison of our results with those of [18] is shown in table 2. As in [18] we choose $R = 2.86$ fm and $d = 0.65$ fm, while the strength of the central potential V_0 is adjusted for each $n-{}^{12}\text{C}$ bound-state energy.

6. Conclusion

In this paper, we have explored an analogy between quantum potential scattering and the classical dynamics of a conservative system of infinite fields. With the aid of an appropriate canonical transformation of a classical Hamiltonian, we were able to derive the Calogero equation for the tangent of the phase shift function. This allowed us to obtain a first-order nonlinear differential equation for the so-called scattering length function, whose asymptotic value for large separations supplies the well-known low-energy expansion in terms of the scattering length, effective range and shape parameter for any partial wave. We have applied our theory to obtain these parameters for typical atom–atom systems (long-range interaction) and neutron–nucleus systems (short-range interaction). We reached very good agreements with results obtained through conventional methods like a direct solution of the scattering Schrödinger equation.

Appendix A. Essentials of quantum potential scattering theory

In this appendix, we supply the essentials of quantum scattering theory as required in section 2. We consider the scattering of a particle from a spherically symmetric potential. The extension to the scattering of a spin $-1/2$ particle can be easily formulated by adding a spin–orbit interaction term to the potential. The regular solution of the radial Schrödinger equation describing the scattering by a spherical potential, $V(r) = \frac{\hbar^2}{2m}U(r)$ [9, 10],

$$\left[-\frac{d^2}{dr^2} + U(r) + \frac{l(l+1)}{r^2} \right] \phi_l(k, r) = k^2 \phi_l(k, r) \quad (\text{A.1})$$

can be written as

$$\phi_l(k, r) = u_l(kr)q_l(k, r) + v_l(kr)p_l(k, r), \quad (\text{A.2})$$

where $u_l(kr)$ and $v_l(kr)$ are the Riccati–Bessel and Riccati–Neumann functions, defined in terms of the usual spherical Bessel $j_l(kr)$ and spherical Neumann functions $n_l(kr)$, respectively,

$$u_l(kr) = krj_l(kr), \quad (\text{A.3})$$

$$v_l(kr) = krn_l(kr). \quad (\text{A.4})$$

The functions, $u_l(kr)$ and $v_l(kr)$ are the regular and irregular solutions of the free radial Schrödinger equation:

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} \right] \omega_l(kr) = k^2 \omega_l(kr), \quad (\text{A.5})$$

where $\omega_l(kr)$ is $u_l(r)$ or $v_l(r)$. Clearly the coefficients $q_l(k, r)$ and $p_l(k, r)$ contain all information about the scattering.

Since $\phi_l(k, r) \rightarrow_{r \rightarrow 0} u_l(kr)$, we have the following boundary conditions satisfied by $q_l(k, r)$ and $p_l(k, r)$:

$$q_l(k, r) \rightarrow_{r \rightarrow 0} 1, \quad (\text{A.6})$$

$$p_l(k, r) \rightarrow_{r \rightarrow 0} 0. \quad (\text{A.7})$$

Since the functions $u_l(k, r)$ and $v_l(k, r)$ are linearly independent in the sense that the Wronskian

$$W[v, u] = vu' - v'u = k, \quad (\text{A.8})$$

it follows that $q_l(k, r)$ and $p_l(k, r)$ may be expressed as

$$q_l(k, r) = \frac{1}{k} W[v_l, \phi_l], \quad (\text{A.9})$$

$$p_l(k, r) = -\frac{1}{k} W[u_l, \phi_l]. \quad (\text{A.10})$$

The usual method of obtaining the scattering observables is to integrate the radial equation and adjust the asymptotic form to the following:

$$\phi_l(k, r) \rightarrow \sin\left(kr - l\frac{\pi}{2} + \delta_l(k)\right), \quad (\text{A.11})$$

which allows the extraction of the phase shift function $\delta_l(k)$. All observables can be written in terms of $\delta_l(k)$. For example, the scattering amplitude $f(k, \theta)$ is just

$$f(k, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(1 - \exp[2i\delta_l(k)]) P_l(\cos \theta), \quad (\text{A.12})$$

with the low-energy limit (only $l = 0$)

$$f(k, 0) = \frac{1}{k} \exp(i\delta_0(k)) \sin(\delta_0(k)) = \frac{1}{k \cot \delta_0(k) - ik}, \quad (\text{A.13})$$

where the function $-\frac{\tan \delta_0(k)}{k}$, in the limit of zero energy, is identified with the scattering length.

In the following, we enumerate some useful formulae for the Riccati–Bessel and Riccati–Neumann functions used in the last section.

The Riccati–Bessel function is given by

$$u_l(\rho) = -(-\rho)^{l+1} \left(\frac{1}{\rho} \frac{d}{d\rho} \right)^l j_0(\rho), \quad (\text{A.14})$$

where the spherical Bessel function $j_0(\rho) = \frac{\sin \rho}{\rho}$, and $\rho = kr$. Similar relation holds for the Riccati–Neumann function

$$v_l(\rho) = -(-\rho)^{l+1} \left(\frac{1}{\rho} \frac{d}{d\rho} \right)^l n_0(\rho), \quad (\text{A.15})$$

where the spherical Neumann function $n_0(\rho) = \frac{\cos \rho}{\rho}$.

The recursion relation follows

$$\omega_l(\rho) = (2l + 1) \frac{\omega_{l+1}(\rho)}{\rho} - \omega_{l-1}(\rho), \quad (\text{A.16})$$

where $\omega_l(\rho)$ stands for $u_l(\rho)$ or $v_l(\rho)$. For the $l = 1$ partial wave, we have

$$u_1(\rho) = \frac{\sin \rho}{\rho} - \cos \rho \quad (\text{A.17})$$

and

$$v_1(\rho) = \frac{\cos \rho}{\rho} + \sin \rho. \quad (\text{A.18})$$

For higher values of l , these functions are easily obtained from the recursion relation above.

Finally, the behaviour of these functions for small values of the argument is

$$u_l(\rho \rightarrow 0) = \frac{\rho^{l+1}}{(2l + 1)!!} \quad (\text{A.19})$$

and

$$v_l(\rho \rightarrow 0) = \frac{(2l - 1)!!}{\rho^l}. \quad (\text{A.20})$$

Appendix B. Charged particle scattering

When the scattering particles are charged, the $\frac{1}{r}$ Coulomb interaction has to be added to the potential. The free solutions are now Coulomb wavefunctions, and special care must be taken when performing the low-energy expansion to ensure convergent results for the scattering length, effective range and shape parameters.

We should emphasize at this point that we leave out all together cases involving long range polarization potentials together with the Coulomb interaction, such as encountered in low-energy scattering of protons from the easily dipole polarizable deuteron. Such a situation also occurs in ionized atom–ionized dimolecule scattering. For more information on the low-energy nuclear p–D scattering problem, we refer the reader to [6–8] and references therein. In these articles, a rigorous discussion about the limitation of the effective range expansion in such cases is given, among other things, in the context of the Calogero equation. In the following we only treat the Coulomb-modified cases which do not present the problems mentioned in [6–8].

The appropriate low-energy expansion was developed in [5], and the quantity $D_l(E)$, becomes in this case

$$D_l^c(E) = \frac{\pi}{2} \exp(2\pi \eta) \tan \delta_l(E), \quad (\text{B.1})$$

where η is the Sommerfeld parameter defined in terms of the charges of the two particles Z_1 and Z_2 , by $\eta = \frac{Z_1 Z_2 e^2}{\hbar v}$, with v being the asymptotic relative velocity. The low-energy expansion is then given by

$$2 \frac{\omega_l(E)}{(l!)^2 a_N^{2l+1}} \left[\frac{2}{D_l^c(E)} + h(\eta) \right] = -\frac{1}{a_l} + \frac{1}{2} r_l k^2 - P_l r_l^3 k^4 + O(k^6). \quad (\text{B.2})$$

In the above, the functions $\omega_l(E)$ and $h(\eta)$ are, respectively

$$\omega_l(E) = \prod_{n=1}^l \left(1 + \frac{n^2}{\eta^2} \right), \quad (\text{B.3})$$

$$h(\eta) = \frac{1}{12\eta^2} + \frac{1}{120\eta^4} + O\left(\frac{1}{\eta^6}\right), \quad (\text{B.4})$$

and a_N is the so-called nuclear Bohr radius, $a_N = \frac{\hbar^2}{\mu Z_1 Z_2 e^2}$, with μ being the reduced mass. The above equation does indeed give convergent results as η goes to ∞ in the zero- E limit. Further, the equation reduces to that for neutral particles upon setting $\eta = 0$.

The corresponding Calogero equation then follows by use of the Wronskian of the scaled Coulomb wavefunctions

$$W[\mathcal{G}_l(kr), \mathcal{F}_l(kr)] = \frac{\pi}{2}, \quad (\text{B.5})$$

where $\mathcal{F}_l(kr)$ and $\mathcal{G}_l(kr)$ are related to the regular, $F_l(kr)$, and irregular, $G_l(kr)$, Coulomb wavefunctions [19]:

$$\mathcal{F}_l(kr) = k^{-1/2} \exp(\pi\eta) F_l(kr), \quad (\text{B.6})$$

and

$$\mathcal{G}_l(kr) = \frac{\pi}{2} k^{-1/2} \exp(-\pi\eta) G_l(kr). \quad (\text{B.7})$$

The ‘Hamiltonian’ function is

$$H(q_l, p_l, r) = \frac{U(r)}{\pi} (\mathcal{F}_l q_l + \mathcal{G}_l p_l)^2. \quad (\text{B.8})$$

The Calogero equation for the tangent function can be derived following the same procedure as that used for the neutral particle scattering:

$$\frac{da_l^c(k, r)}{dr} - \frac{\pi}{2} \exp[-2\pi\eta] U(r) \left[\mathcal{F}_l(kr) - \frac{\pi}{2} \exp[-2\pi\eta] \mathcal{G}_l(kr) a_l^c(k, r) \right]^2 = 0, \quad (\text{B.9})$$

where $a_l^c(k, \infty)$ is just the Coulomb-modified tangent function, $D_l^c(E) = \frac{\pi}{2} \exp(2\pi\eta) \tan \delta_l(E)$. Clearly, once this function is calculated, the low-energy parameters can be obtained from the expression $2 \frac{\omega_l(E)}{(l!)^2 a_N^{2l+1}} \left[\frac{2}{D_l^c(E)} + h(\eta) \right] = -\frac{1}{a_l} + \frac{1}{2} r_l k^2 - P_l r_l^3 k^4 + O(k^6)$, above.

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