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Effective-range theory in two dimensions^{a)}

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A parametrization of low-energy two-dimensional quantum scattering is given which is in the tradition of familiar three-dimensional effective-range theory. A scattering length differing from previous treatments is introduced whose behavior reflects the repulsive or attractive nature of the interaction, and whether or not bound states are present. However its definition is subject to an unknown length parameter. An effective-range parameter is also defined and together with the scattering length explains the nonexistence of the Efimov effect in two dimensions. It is also shown that the Ramsauer–Townsend effect exists in 2D. Application to the case of a square-well potential reveals direct relationships between the unknown length parameter and the effective range to the actual range of the potential.

I. INTRODUCTION

Over the past few years there has been considerable interest in two-dimensional (2D) systems such as helium adsorbed on graphite¹ and spin-polarized hydrogen ($H\downarrow$) recombining on a helium film.² The theoretical treatment of such systems involves 2D quantum scattering theory, and in particular the low-energy behavior of quantities such as the scattering phase shifts. It is therefore useful to have a parametrization of these quantities, and recently two rather different treatments have appeared in the literature.^{3,4}

Our purpose here is to propose a third parametrization which we believe remains closer to the physics of the situation, and thus is more in keeping with the spirit of the original effective-range expansion introduced for three-dimensional (3D) scattering.^{5–7} A crucial point in our treatment is the appearance of an arbitrary quantity R with the dimension of length. From a purely mathematical point of view its value is not of great importance (it could be set equal to unity), but it is important for the physical interpretation of the scattering process, and so we devote some attention to a proper choice of R .

In 3D, the low-energy behavior of the s -wave scattering phase shift $\delta = \delta_0(k)$ is conventionally parametrized by the expansion

$$k \cot \delta = -1/a + \frac{1}{2}r_0 k^2 + O(k^4), \quad (1)$$

where k^2 is the relative energy in units of $\hbar^2/2\mu$, μ is the reduced mass, a the scattering length, and r_0 the effective range. In 2D, we do not have an exact analog of Eq. (1), since $\cot \delta$ diverges logarithmically when $k \rightarrow 0$. This can already be seen in the hard-disk case,⁸ where

$$\pi/2 \cot \delta = \ln[kd/2] + C + \frac{1}{4}d^2 k^2 + O(k^4) \quad (2)$$

with d being the hard-disk radius and $C = 0.5772\dots$ the Euler constant. The problem is to modify Eq. (2) to cover the case where the particles interact via a general short-range potential. If the potential has a finite range R_C , this can be

achieved, to lowest order in k , by making the replacement

$$d \rightarrow b = R_C \exp\{-1/[R_C L_O(R_C)]\} \quad (3)$$

in the logarithmic term of Eq. (2). Here $L_O(R_C)$ is the logarithmic derivative of the wave function evaluated at R_C [i.e., $L(R_C)$] for zero energy. Such a procedure was used by Bruch^{9,10} to generalize hard-disk results, and the recent papers of Verhaar *et al.*⁴ advocate using what is essentially b as the 2D scattering length, the coefficient of k^2 still remains associated with the effective range.

The definition of Bolle and Gesztesy³ does not place the scattering length in the logarithm, and is closer to the usual 3D definition. We shall comment further on these approaches below, after giving our own treatment.

II. 2D EFFECTIVE-RANGE EXPANSION

To find the low-energy behavior of the two-body s -wave scattering phase shift in 2D we start by showing that the general expression for it can be derived following the method of Bethe.^{6–11} Accordingly, we write down the reduced radial wave function $u(r)$ for the interacting system

$$\frac{d^2 u}{dr^2} + [k^2 - V(r) + 1/\{4r^2\}]u = 0, \quad (4)$$

where $V(r)$ is the potential. For the noninteracting system and in the asymptotic region, this becomes

$$\frac{d^2 v}{dr^2} + [k^2 + 1/\{4r^2\}]v = 0. \quad (5)$$

Equation (5) has as solutions the Bessel functions J_0, N_0 of zero order, and we choose the combination

$$v(r) = \pi/2 \sqrt{r} [-\cot \delta J_0(kr) + N_0(kr)]. \quad (6)$$

For the solution of Eq. (4), we impose boundary conditions $u(0) = 0$ and $u(r) \approx v(r)$ as $r \rightarrow \infty$.⁵ If we let u_1, u_2 , be the solutions of Eq. (4) at energies k_1^2, k_2^2 and let v_1, v_2 , be the corresponding solutions of Eq. (5), then, in standard fashion, we can derive the expression

$$\begin{aligned} & [v_2 v_1' - v_1 v_2']_{r_<}^{r_>} - [u_2 u_1' - u_1 u_2']_{r_<}^{r_>} \\ & = \{k_2^2 - k_1^2\} \\ & \times \int_{r_<}^{r_>} [v_1 v_2 - u_1 u_2] dr. \end{aligned} \quad (7)$$

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This is to be evaluated in the limit $r_{<} \rightarrow 0$, $r_{>} \rightarrow \infty$, using the boundary conditions on $u(r)$, and the small r behavior of $v(r)$ which from Eq. (6) is

$$v(r) \approx \frac{\pi}{2} \sqrt{r} \{ -\cot \delta + \frac{2}{\pi} [C + \ln(kr/2)] \}, \quad r \rightarrow 0.$$

We find

$$\begin{aligned} & \{ \frac{\pi}{2} \cot \delta(k_2) - [C + \ln(k_2 r_{<}/2)] \} \\ & - \{ \frac{\pi}{2} \cot \delta(k_1) - [C + \ln(k_1 r_{<}/2)] \} \\ & \approx \{ k_2^2 - k_1^2 \} \int_{r_{<}}^{\infty} [v_1 v_2 - u_1 u_2] dr, \quad r_{<} \rightarrow 0. \end{aligned} \quad (7')$$

We wish to emphasize that the r dependence of the left-hand side vanishes, and in fact we can write

$$\ln[k_1 r_{<}/2] - \ln[k_2 r_{<}/2] = \ln[k_1 R/2] - \ln[k_2 R/2],$$

where R is an arbitrary quantity with the dimension of length. Making this replacement in Eq. (7), using the solution of Eq. (5) for $k = 0$, and letting $k_1 \rightarrow 0$, $k_2 \rightarrow k$, we obtain

$$\begin{aligned} F(R) &= \frac{\pi}{2} \cot \delta - [C + \ln(kR/2)] \\ &= -K + \frac{1}{4} r_0^2 k^2 + \dots, \end{aligned} \quad (8)$$

where

$$K = -\lim_{k \rightarrow 0} \{ \frac{\pi}{2} \cot \delta - [C + \ln(kR/2)] \} \quad (9)$$

and

$$r_0^2 = 4 \int_0^{\infty} (v_0^2 - u_0^2) dr, \quad (10)$$

where v_0 and u_0 denote v and u at $k = 0$. We stress that it is necessary to introduce R in order to prevent a discontinuity in physical dimension.⁴ Bolle and Gesztesy have ignored R in composing their effective-range expression, at worst introducing the dimensional inconsistency just mentioned and at best willy-nilly setting it to unity; we claim that R must be properly assigned a value and a dimension. We discuss this in the next section.

III. THE MATCHING PARAMETER R AND OTHER SCATTERING PARAMETERS

To bolster our contention that the parameter R is an important quantity in 2D scattering we considered a general potential with a cutoff at R_c or any short-range potential for which R_c designates the beginning of the asymptotic region. Then the 2D s -wave phase shift satisfies

$$\begin{aligned} \cot \delta &= [k N'_0(kR_c) - L(R_c) N_0(kR_c)] / \\ & [k J'_0(kR_c) - L(R_c) J_0(kR_c)], \end{aligned} \quad (11)$$

where the prime denotes a derivative with respect to the argument. Then we find, after simplifying and taking kR_c to be small, that

$$\begin{aligned} F(R_c) &= \frac{\pi}{2} \cot \delta - [C + \ln(kR_c/2)] \\ &= -1/[R_c L_0(R_c)] + O(k^2). \end{aligned} \quad (12)$$

It seems obvious by comparing Eq. (8) and Eq. (12) that the natural choice for R is not unity but R_c while K is $1/[R_c L_0(R_c)]$.

In direct analogy to the case in 3D [see Eq. (1)], we refer to r_0 in Eq. (8) as the 2D effective range, which is uniquely defined and has the dimension of length. We are in agreement with Verhaar *et al.* and Bolle and Gesztesy on this. It is a different situation with the definition of the scattering length which must reside in K and depends on the choice of R .

Verhaar *et al.* have effectively absorbed K into the logarithmic term in Eq. (8) in order to define $a = R \exp[-K]$, hereafter labeled a_V , as the scattering length and reduce the number of parameters in that equation to two. This is perhaps satisfactory for potentials which do not differ greatly from pure repulsion, but for more general potentials it is desirable to have a scattering length which reflects some of the physics of the situation, such as the change from a predominantly repulsive to a predominantly attractive potential, and the appearance of new bound states at certain potential strengths, i.e., one would prefer a_V to be sensitive in the topological sense to these changes. The definition of Verhaar *et al.* fails in this regard since a_V is a relatively innocuous function.

There are now really two good choices for the definition of the scattering length, viz. (1) $a = K$, and (2) $a = K^{-1}$ which we shall label as a_{AGL} and a'_{AGL} , respectively, and are dimensionless. (In truth there are two other choices, $a = RK$, and $a = RK^{-1}$, should one wish to define an a with the dimension of length.) Choice (2) is Bolle and Gesztesy's selection with R simultaneously set to unity which we label a_{BG} .

For the purposes of illustration and clarification of the relative effectiveness of a_{AGL} and a'_{AGL} we consider the case of a square-well potential of depth β^2 and width R_c . The effective-range expansion becomes

$$\begin{aligned} F(R_c) &= -1/L_0(\beta R_c) + \{ R_c^2/4 - R_c^2/[2L_0(\beta R_c)] \\ & - 1/(2\beta^2) \} k^2 + O(k^4), \end{aligned} \quad (13)$$

where $L_0(x) = x J'_0(x)/J_0(x)$. Thus the natural identification here is

$$\begin{aligned} R &= R_c, \\ K &= 1/L_0(\beta R_c), \\ r_0^2 &= R_c^2 - 2R_c^2/L_0(\beta R_c) - 2/\beta^2. \end{aligned} \quad (14)$$

We remark that each of a_{AGL} and a'_{AGL} , as defined in Eq. (14), has a behavior which is qualitatively similar to the usual scattering length for a 3D square well. (See Fig. 1.) Each is positive for a repulsive well, goes negative as the potential becomes attractive, and has alternating zeros and poles as the potential strength is increased. The main difference is that the zeros of a'_{AGL} correspond to the introduction of new bound states whereas it is the poles of a_{AGL} at these points, in harmony with 3D. That a_{AGL} is given in terms of the inverse of a logarithmic derivative also brings it closer to the familiar 3D form.⁷ On the other hand it is a'_{AGL} that follows the 3D plot more closely. It is clear that because of essential differences between 2D and 3D scattering, such as the divergence of the zero-energy cross section in the former, it is impossible to define parameters which are exact analogs. Thus although a_{AGL} and a'_{AGL} are superior to a_{BG} and a_V , it

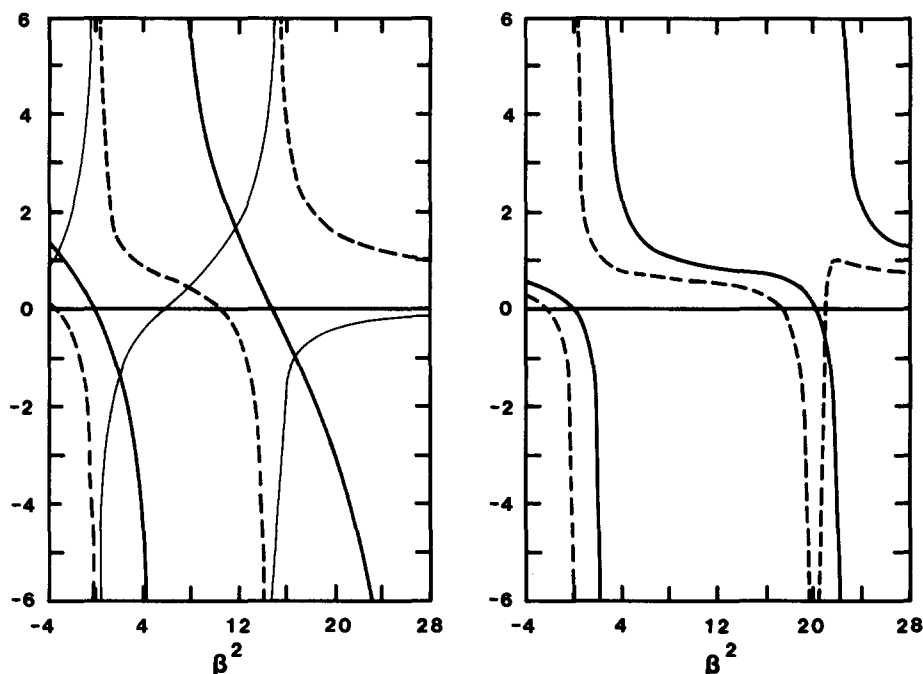


FIG. 1. (a) a_{AGL} (thin solid line), a'_{AGL} (thick solid line), and r_0 (dash line) for a square well in two dimensions; (b) a (solid line), and r_0 (dash line) for a square well in three dimensions. In each case the well has width 1 and depth β^2 .

is difficult to pick between the former pair.

The effective range r_0 also shows certain similarities to its 3D counterpart, though again there are differences; e.g., it tends to infinity rather than the range of the potential at potential strengths which introduce a new bound state.

For an infinitely repulsive square well, a'_{AGL} is infinite, a_{AGL} is zero, and r_0 is R while in 3D the scattering length is R with the effective range equal to $\frac{1}{3}R$.

Another difference between 2D and 3D becomes apparent if we look at the limit of r_0 as $|K| \rightarrow 0$ (the so-called “intrinsic range”⁵): in 3D this limit is simply R , the actual range of the well, but in 2D we find

$$\lim_{|K| \rightarrow 0} r_0^2 = R^2 - 2/\beta^2 = R^2 [1 - 2/x_i^2], \quad (15)$$

where we have used the fact that $|K|$ becomes zero where $\beta R = x_i$, the i th zero of $J_0(x)$. Thus the intrinsic range in this case depends on the number of bound states the potential supports.

We see that if $|K| \gg 1$, r_0^2 will become large and even negative, so it is no longer possible to relate r_0 to the actual potential range. Then it is better to use the inverse expansion (cf. Ref. 12 where the corresponding discussion is given for the 3D case):

$$F(R)^{-1} = -K^{-1} + \frac{1}{2}K^{-1}[R^2 + K^{-1}/\beta^2 - \frac{1}{2}K^{-1}R^2]k^2 + O(k^4). \quad (16)$$

This shows that the general inverse expansion should have the form

$$F(R)^{-1} = -K^{-1} + \frac{1}{2}K^{-1}\bar{r}_0^2 k^2 + \dots, \quad (17)$$

where \bar{r}_0 will be related to the potential range.

In summary it should be noted that the presence of R in our effective-range expansion pushes the number of parameters up to three; the usual linear plot of functionals of δ and k can only yield a fix on two! However R and K need not be coupled together as was done by Verhaar *et al.* Whenever explicit values for R and K are needed, a suitable approximation would be to take $R = R_c$ if available. Otherwise a reasonable guesstimate is sufficient. We have solved the 2D Schrödinger equation numerically for the phase shifts of the Lennard-Jones potential $\{V(r) = 4\epsilon[(\sigma/r)^6 - (\sigma/r)^{12}]\}$ representing various systems¹³ with different values of the de Boer parameter $\eta = \hbar^2/m\epsilon\sigma^2$ and subsequently extracted K and r_0 for a range of values of R without detecting any great sensitivity to R . (See Table I. Note that r_0^2 is always positive in all the examples.)

The connection between bound states and scattering length can also be seen from the relation derived similarly to Eq. (8),

$$K = C + \ln[\kappa R/2] - \frac{1}{4}r_0^2\kappa^2 + \dots, \quad (18)$$

where $\kappa^2 (>0)$ is the energy of a bound state lying near the continuum. Its form verifies the behavior of the binding en-

TABLE I. 2D scattering length and effective range for various molecular systems.

Atomic species	Status of two-body system	R (Å)	r_0 (Å)	a_{AGL}	a'_{AGL}	a_{BG}	a_V
H ₂	unbound	10	6.0	2.1	0.47	-5.5	1.20
D ₂	just unbound	10	76.9	19.3	0.05	0.06	4.4-8
³ He	just bound	5.5	109	6.5	0.15	0.21	8.3-3
		10		7.1	0.14	0.21	8.2-3
⁴ He	very bound	5.5	16.2	-1.6	-0.63	-0.30	27.2
		10		1.6	-1.05	-0.31	25.9

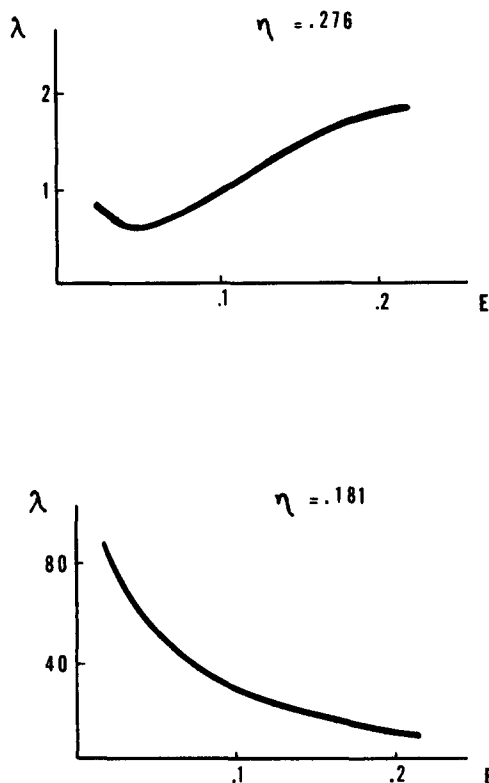


FIG. 2. (a) The cross length (from the s -wave contribution only) plotted against energy for the system near threshold whose de Boer parameter $\eta = 0.276$ ($\eta = 0.271$ at threshold); (b) same as for (a) except for the system whose $\eta = 0.181$.

ergy of a 2D system near threshold¹⁴ and will be valid only if the potential is sufficiently short-range, this requirement being also necessary in the 3D case.¹⁵

Our final remark for this section concerns the effective-range expansion for the p -wave case, where we find the form

$$k^2 \cot \delta_1 = -K_1 + 2/\pi [C + \ln(kR/2)]k^2 + \frac{1}{2}r_1k^2 + \dots \quad (19)$$

The scattering length, embedded in K_1 , is now uniquely defined but the range r_1 depends on the choice of R and is dimensionless.

IV. APPLICATIONS OF THE THEORY

The Ramsauer-Townsend effect does occur in 2D. Our analysis of the cross length, the 2D analog of the 3D cross section and sporting length units (e.g., for s and p waves, the expressions for this quantity are $\lambda_0 = 4/k \cdot \sin^2 \delta$ and $\lambda_1 = 8/k \cdot \sin^2 \delta_1$),^{8,16} indicates that the effect is manifest when $|K|$ is large, i.e., when the interaction is such as to be near the region for a bound state, exactly the same conditions as in one dimension but different from 3D.¹³ (See Fig. 2.)

Having presented four selections for the 2D scattering length from the effective-range expansion, Eq. (8), we now state that each can provide a ready explanation for nonexist-

tence of the Efimov effect for three bosons in 2D. At the threshold of a new two-boson bound state, the ratio $|a/r_0|$ is a small finite quantity in all cases. This is in line with the fact that no Efimov states exist in 2D.¹⁷ (In 3D the ratio is infinite at threshold and accounts for the presence of an infinite number of loosely bound three-body states.) An alternative way to approach the same conclusion is to realize that near threshold for the bound two-body state in 2D the cross length has a minimum indicating a small "influence sphere" for the particles while with the same situation in 3D the influence sphere is extremely large and creates the long-range effective interaction which introduces the Efimov states.

Bolle *et al.* have also found some surprises when they considered the applicability of Levinson's theorem in 2D.³ An intimation of this was seen in our analysis of the scattering length and effective range for the Lennard-Jones potentials; the behavior of all the 2D scattering lengths as a function of η was different from that in 3D. Where Uang and Stwalley⁷ had shown a change in scattering length from $-\infty$ to $+\infty$ as evidence for the appearance of a bound state according to Levinson's theorem, we found no such change in all our a 's.

In conclusion, we feel that the body of recent work exemplified by Refs. 3 and 4 and this work portend exciting developments in the area of 2D physics.

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