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Scattering by a contact potential in three and lower dimensions

Qiong-gui Lin

China Centre of Advanced Science and Technology (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China

and

Department of Physics, Zhongshan University, Guangzhou 510275, People's Republic of China¹

E-mail: qg.lin@163.net and stdp@zsu.edu.cn

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Abstract

We consider the scattering of nonrelativistic particles in three dimensions by a contact potential $\Omega\hbar^2\delta(r)/2\mu r^\alpha$, which is defined as the $a \rightarrow 0$ limit of $\Omega\hbar^2\delta(r-a)/2\mu r^\alpha$. It is surprising that it gives a nonvanishing cross section when $\alpha = 1$ and $\Omega = -1$. When the contact potential is approached by a spherical square well potential instead of the above spherical shell one, one obtains basically the same result except that the parameter Ω that gives a nonvanishing cross section is different. Similar problems in two and one dimensions are studied and results of the same nature are obtained.

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1. Introduction

In this paper we consider a very simple problem, the scattering of nonrelativistic particles by a contact potential, which is nonzero (in general infinite) at one point and vanishes elsewhere. More specifically, in three dimensions we consider the potential

$$V(r) = \frac{\Omega\hbar^2}{2\mu} \frac{\delta(r)}{r^\alpha} \quad (1)$$

where Ω and α are real parameters and μ is the mass of the particle. Since this is somewhat difficult to handle in practice, we are actually considering the $a \rightarrow 0$ limit of the spherical shell potential

$$V_a(r) = \frac{\Omega\hbar^2}{2\mu} \frac{\delta(r-a)}{r^\alpha} = \frac{\Omega\hbar^2}{2\mu} \frac{\delta(r-a)}{a^\alpha} \quad (2)$$

where $a > 0$, which is better defined. The latter is a contact potential since in the limit it is nonvanishing (and infinite if $\alpha \geq 0$) only at $r = 0$, though one may think it is different from

¹ Address for correspondence.

the former. The interest of such a problem is threefold. First, according to classical mechanics, the scattering cross section for a contact potential in three or two dimensions is obviously zero. In one dimension an incident particle would be bounced back by a contact potential (total reflection) if the potential were infinite at the nonvanishing point. However, the case may be different in quantum mechanics. Second, if a finite cross section is possible in quantum mechanics, one may think that a ‘larger’ infinity (higher singularity) at the nonvanishing point would give a larger cross section, but this turns out to be incorrect. Only a ‘proper’ infinity gives a nonvanishing result. For the above potential, a nonvanishing cross section is obtained only when $\alpha = 1$ and $\Omega = -1$. Third, an exact result is easily available. This is because all phase shifts except δ_0 vanish in the limit $a \rightarrow 0$, which is what is expected for a contact potential.

In the next section we consider the above problem in three dimensions. Instead of the spherical shell potential (2), the contact potential (1) can be approached by some other potential as well. It is then of interest to see whether the same result is obtained. A simple candidate is the square well potential. This is also considered. It turns out that the result is basically the same, except that the parameter Ω that gives a nonvanishing cross section is different.

In section 3 we consider a similar problem in two dimensions. It turns out that the potential of the same form as in three dimensions gives a vanishing cross section for any α and Ω . We then consider the $a \rightarrow 0$ limit of the circular ring potential

$$V_a(r) = \frac{\Omega \hbar^2}{2\mu} \frac{\delta(r-a)}{r^\alpha [-\ln(r/a_0)]^\beta} = \frac{\Omega \hbar^2}{2\mu} \frac{\delta(r-a)}{a^\alpha [-\ln(a/a_0)]^\beta} \quad (3)$$

where a_0 is a length scale and β is another real parameter. We take $a_0 > a$ (note that we would finally take the limit $a \rightarrow 0$) such that $-\ln(a/a_0)$ is positive. It turns out that a nonvanishing cross section is obtained only when $\alpha = 1$, $\beta = 1$ and $\Omega = -1$. We also consider a square well potential that approaches the same contact potential. It turns out that all results are exactly the same as for the above circular ring potential. This is somewhat different from the case in three and one dimensions. In section 4 we consider the $a \rightarrow 0$ limit of the double delta potential in one dimension:

$$V_a(x) = \frac{\Omega \hbar^2}{2\mu} \frac{\delta(x-a) + \delta(x+a)}{|x|^\alpha} = \frac{\Omega \hbar^2}{2\mu} \frac{\delta(x-a) + \delta(x+a)}{a^\alpha} \quad (4)$$

where $a > 0$. When $\alpha = 0$, this tends to the ordinary $\delta(x)$ potential and we indeed obtain the known result [1], which is already different from the classical one. Here we are interested in the results for other values of α . It turns out that $\alpha < 0$ leads to total transmission. This is an expected result since there is no singularity in this case. When $\alpha > 0$ one has in general total reflection. This is also expected since the singularity is strong. What is unexpected is, however, when $\alpha = 1$ and $\Omega = -1$ one has total transmission with a phase shift π . When the contact potential is approached by a square well potential, the result is roughly the same. However, in addition to the total transmission with a phase shift π for some specific values of Ω (not -1), we have true total transmission for some other values of Ω .

2. Three dimensions

Consider scattering in three dimensions by the spherically symmetric potential (2). If a is a constant, this is the ordinary spherical shell potential studied in the literature [1], and the parameter α plays no role. However, here we are interested in the limit $a \rightarrow 0$, so different α would lead to different results. The radial equation for the l th partial wave is

$$R''(r) + \frac{2}{r}R'(r) + \left[k^2 - \frac{l(l+1)}{r^2} \right] R(r) - \frac{\Omega}{a^\alpha} R(a)\delta(r-a) = 0 \quad l = 0, 1, 2, \dots \quad (5)$$

where $k = \sqrt{2\mu E}/\hbar$ and $E > 0$ is the energy of the incident particle. The solution of this equation is

$$R(r) = A_l j_l(kr) \quad r < a \quad (6a)$$

$$R(r) = \cos \delta_l j_l(kr) - \sin \delta_l n_l(kr) \quad r > a \quad (6b)$$

where δ_l is the phase shift, A_l is a constant and j_l and n_l are the spherical Bessel and Neumann functions, respectively. The two parts of the solution must be appropriately connected at $r = a$. The connection conditions are

$$R(a^+) = R(a^-) \quad (7a)$$

$$R'(a^+) - R'(a^-) = \frac{\Omega}{a^\alpha} R(a) \quad (7b)$$

where $a^\pm = a \pm 0$. Equation (7b) is obtained by integrating equation (5) from a^- to a^+ . Since the jump of $R'(r)$ at $r = a$ is finite we have equation (7a). The phase shift is determined by these conditions and the result is

$$\tan \delta_l = \frac{b\xi j_l^2(\xi)}{-\xi^{\alpha-1} + b\xi j_l(\xi)n_l(\xi)} \quad (8)$$

where $\xi = ka$ and $b = \Omega k^{\alpha-1}$. The scattering amplitude is given in many textbooks of quantum mechanics as

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [\exp(2i\delta_l) - 1] P_l(\cos \theta). \quad (9)$$

Though we have an analytic expression for the phase shifts, it is difficult to have a closed result for the scattering amplitude since the summation in equation (9) cannot be worked out. Here we are only interested in the limit $a \rightarrow 0$ (or $\xi \rightarrow 0$), however, so the problem is much simpler. If $\alpha > 1$, the first term in the denominator of equation (8) can be neglected in comparison with the second, so we have obviously $\tan \delta_l \rightarrow 0$ for all l and $f(\theta) \rightarrow 0$. If $\alpha < 1$ (including negative α), the second term in the denominator can be neglected in comparison with the first, and the same result is easily achieved. If $\alpha = 1$, the two terms in the denominator are of the same order. One should be careful in this case. Obviously, the numerator behaves like ξ^{2l+1} , while the denominator behaves like ξ^0 or, if b takes some specific value, like ξ^2 , so if $l \geq 1$, we have $\tan \delta_l \rightarrow 0$. A nonvanishing phase shift is therefore possible only when $l = 0$, as expected for a contact potential. If $l = 0$ and $b \neq -1$, we have $\tan \delta_0 \rightarrow 0$ as well, and thus $f(\theta) \rightarrow 0$. If $b = -1$, however, we have $\tan \delta_0 \sim 3/2\xi \rightarrow \infty$, so that $\delta_0 = \pi/2, \text{ mod } \pi$. Only in this case do we have a nonvanishing scattering amplitude

$$f(\theta) = \frac{i}{k} \quad (10)$$

which is of course independent of θ . The differential and total cross sections are

$$\sigma(\theta) = \frac{1}{k^2} = \frac{\hbar^2}{\mu^2 v^2} \quad \sigma_t = \frac{4\pi}{k^2} = \frac{4\pi\hbar^2}{\mu^2 v^2} \quad (11)$$

where v is the classical velocity of the incident particle. Therefore only a contact potential with proper singularity and proper strength gives a nontrivial result. We make some remarks. First, the result is inversely proportional to the incident energy. Second, $b = -1$ yields $\Omega = -1$ since $\alpha = 1$. Third, when $\alpha = 1$, $\tan \delta_0$ depends only on $\xi = ka$ (not on k and a separately), so that $\lim_{a \rightarrow 0} \tan \delta_0 = \infty$ for finite k implies $\lim_{k \rightarrow 0} \tan \delta_0 = \infty$ for finite a . According to the analysis of the Levinson theorem [2-5], one has in general $\lim_{k \rightarrow 0} \tan \delta_0 = 0$; only when

there exists a half-bound state [6] with zero energy and $l = 0$ does the limit become infinite. In fact, the zero-energy solution with $l = 0$ to equation (5) is

$$R(r) = 1 \quad r < a \quad (12a)$$

$$R(r) = B_0 r^{-1} \quad r > a \quad (12b)$$

where B_0 is a constant. The two parts of the solution can be connected by the conditions (7) only when $\Omega = -1$. This is consistent with the above result. The solution (12) is called a half-bound state because it tends to zero at infinity but is not normalizable.

As pointed out in section 1, the contact potential can be approached by some potential other than the above spherical shell one. It is then of interest to see whether the same conclusion is achieved. We consider the spherical square well potential ($\Omega < 0$ is assumed for such potentials in all dimensions)

$$V^a(r) = \begin{cases} 3\Omega\hbar^2/2\mu a^{\alpha+1} & r < a \\ 0 & r > a. \end{cases} \quad (13)$$

This gives the integration $\int V^a(r) d^3x = 2\pi\Omega\hbar^2/\mu a^{\alpha-2}$, the same as given by the spherical shell potential (2). Thus when $a \rightarrow 0$ they would tend to the same contact potential. The phase shifts for this potential can be easily found. They are determined by

$$\tan \delta_l = \frac{\eta j_l(\xi) j_{l+1}(\eta) - \xi j_{l+1}(\xi) j_l(\eta)}{\eta n_l(\xi) j_{l+1}(\eta) - \xi n_{l+1}(\xi) j_l(\eta)} \quad (14)$$

where ξ is defined as before, and $\eta = \sqrt{\xi^2 - 3b\xi^{1-\alpha}}$. Then we let $\xi \rightarrow 0$ and analyse the behaviour of the phase shifts. After careful calculations, it is found that $\tan \delta_l \rightarrow 0$ for all l if $\alpha \neq 1$. Thus a nontrivial result is possible only when $\alpha = 1$, the same conclusion as before. If $\alpha = 1$, it can be shown that $\tan \delta_l \rightarrow 0$ for all $l \neq 0$. As for $l = 0$, we have in general $\tan \delta_0 \rightarrow 0$, except when $j_{-1}(\sqrt{-3b}) = 0$ or $n_0(\sqrt{-3b}) = 0$. In the latter case we have $\tan \delta_0 \sim \xi^{-1} \rightarrow \infty$, and hence the nontrivial results (10) and (11). The above condition is equivalent to $\cos(\sqrt{-3b}) = 0$ or (note that $\alpha = 1$)

$$\Omega = -\frac{(2N-1)^2\pi^2}{12} \quad (15)$$

where N is a natural number. The difference from the previous case is that for the spherical shell potential there is only one specific value of Ω that leads to a nontrivial cross section while in the present case we obtain a series of such values (but the condition $\alpha = 1$ is the same). This difference is related to the different situation for the appearance of half-bound states with $l = 0$ (for $\alpha = 1$ and finite a). For the spherical shell potential the half-bound state can appear only once when $\Omega = -1$, while for the square well potential it can appear many times when Ω takes on the above values.

3. Two dimensions

In this section we consider a similar problem in two dimensions. We still use (r, θ) for the polar coordinates on the xy plane. These should not be confused with those in three dimensions. If one considers a potential of the form (2), it can be shown that the result is trivial in the limit $a \rightarrow 0$. So we consider the potential (3). The radial wave equation for the m th partial wave is

$$R''(r) + \frac{1}{r}R'(r) + \left(k^2 - \frac{m^2}{r^2}\right)R(r) - \frac{\Omega}{a^\alpha[-\ln(a/a_0)]^\beta}R(a)\delta(r-a) = 0 \quad (16)$$

$$m = 0, 1, 2, \dots$$

The solution of this equation is

$$R(r) = C_m J_m(kr) \quad r < a \quad (17a)$$

$$R(r) = \cos \delta_m J_m(kr) - \sin \delta_m N_m(kr) \quad r > a \quad (17b)$$

where δ_m is the phase shift, C_m is a constant and J_m and N_m are the ordinary Bessel and Neumann functions, respectively. The connection conditions at $r = a$ are

$$R(a^+) = R(a^-) \quad (18a)$$

$$R'(a^+) - R'(a^-) = \frac{\Omega}{a^\alpha [-\ln(a/a_0)]^\beta} R(a). \quad (18b)$$

The phase shift is determined by these conditions and the result is

$$\tan \delta_m = \frac{b\pi J_m^2(\xi)}{-2\xi^{\alpha-1}[-\ln(\xi/\xi_0)]^\beta + b\pi J_m(\xi)N_m(\xi)} \quad (19)$$

where $\xi = ka$, $\xi_0 = ka_0$ and $b = \Omega k^{\alpha-1}$. The scattering amplitude is given by [7]

$$f(\theta) = -\frac{i}{\sqrt{2\pi k}} \sum_{m=-\infty}^{+\infty} [\exp(2i\delta_m) - 1] e^{im\theta}. \quad (20)$$

As before we do not attempt to study the general case in detail, but are interested in the limit $a \rightarrow 0$ (or $\xi \rightarrow 0$) only. If $\alpha > 1$, the first term in the denominator of equation (19) can be neglected in comparison with the second, so we have obviously $\tan \delta_m \rightarrow 0$ for all m and $f(\theta) \rightarrow 0$. If $\alpha < 1$ (including negative α), the second term in the denominator can be neglected in comparison with the first, and the same result is easily achieved. Therefore a nontrivial result is possible only when $\alpha = 1$. In this case

$$\tan \delta_m = \frac{b\pi J_m^2(\xi)}{-2[-\ln(\xi/\xi_0)]^\beta + b\pi J_m(\xi)N_m(\xi)}. \quad (21)$$

If $m \geq 1$, the numerator behaves like ξ^{2m} , while the denominator behaves like ξ^0 if $\beta < 0$ or like $[-\ln(\xi/\xi_0)]^\beta$ if $\beta > 0$ (note that the case $\beta = 0$ leads to a trivial result, which has been mentioned at the beginning of this section), so if $m \geq 1$, we have $\tan \delta_m \rightarrow 0$. A nonvanishing phase shift is therefore possible only when $m = 0$, as expected for a contact potential. If $m = 0$, the numerator behaves like ξ^0 , while the denominator behaves like $\ln \xi$ if $\beta < 1$ or like $[-\ln(\xi/\xi_0)]^\beta$ if $\beta > 1$. So if $\beta \neq 1$ we have $\tan \delta_0 \rightarrow 0$ as well, and thus $f(\theta) \rightarrow 0$. If $\beta = 1$ but $b \neq -1$, the denominator still behaves like $\ln \xi$, so we still have $\tan \delta_0 \rightarrow 0$, and thus $f(\theta) \rightarrow 0$. However, if $\beta = 1$ and $b = -1$, we have in the limit $a \rightarrow 0$

$$\tan \delta_0 = \frac{\pi}{2\gamma + 2\ln(\xi_0/2)} \quad (22)$$

where γ is Euler's constant, and in this case we have a nonvanishing scattering amplitude

$$f(\theta) = \sqrt{\frac{2\pi}{k}} \frac{1}{2\gamma + 2\ln(\xi_0/2) - i\pi} \quad (23)$$

which is of course independent of θ , but note that the result depends on a_0 or ξ_0 . The differential and total cross sections are

$$\sigma(\theta) = \frac{2\pi}{k[4(\gamma + \ln(\xi_0/2))^2 + \pi^2]} = \frac{2\pi\hbar}{\mu v[4(\gamma + \ln(\xi_0/2))^2 + \pi^2]} \quad (24)$$

$$\sigma_t = \frac{4\pi^2}{k[4(\gamma + \ln(\xi_0/2))^2 + \pi^2]} = \frac{4\pi^2\hbar}{\mu v[4(\gamma + \ln(\xi_0/2))^2 + \pi^2]}. \quad (25)$$

Therefore only when $\alpha = 1$, $\beta = 1$ and $\Omega = -1$ do we obtain a nontrivial result.

As in three dimensions, we then consider the two-dimensional square well potential

$$V^a(r) = \begin{cases} \Omega \hbar^2 / \mu a^{\alpha+1} [-\ln(a/a_0)]^\beta & r < a \\ 0 & r > a. \end{cases} \quad (26)$$

This gives the integration $\int V^a(r) d^2x = \pi \Omega \hbar^2 / \mu a^{\alpha-1} [-\ln(a/a_0)]^\beta$, the same as given by the circular ring potential (3). Thus when $a \rightarrow 0$ they would tend to the same contact potential. The phase shifts for this potential can be easily found. They are determined by

$$\tan \delta_m = \frac{\eta J_m(\xi) J_{m+1}(\eta) - \xi J_{m+1}(\xi) J_m(\eta)}{\eta N_m(\xi) J_{m+1}(\eta) - \xi N_{m+1}(\xi) J_m(\eta)} \quad (27)$$

where ξ is defined as before, and $\eta = \sqrt{\xi^2 - 2b\xi^{1-\alpha} [-\ln(\xi/\xi_0)]^{-\beta}}$. Then we let $\xi \rightarrow 0$ and analyse the behaviour of the phase shifts. The present situation is somewhat more complicated than that in three dimensions. The various cases with different parameter values should be discussed separately. After careful calculations, it is found that the nontrivial results (22)–(25) are obtained only when $\alpha = 1$, $\beta = 1$ and $\Omega = -1$. This is exactly the same conclusion as for the circular ring potential. Note that the nontrivial result in two dimensions has nothing to do with the existence of half-bound states. Thus the situation is rather different from that in three or one dimensions (see below).

4. One dimension

Now we turn to the potential (4) in one dimension. For scattering of particles incident from the left, the boundary conditions are

$$\psi(x) = e^{ikx} + Re^{-ikx} \quad x < -a \quad (28a)$$

$$\psi(x) = Te^{ikx} \quad x > a. \quad (28b)$$

Here R and T are the reflection and transmission amplitudes, respectively. On the other hand, with a given energy (or a given k), there exist two linearly independent solutions to the Schrödinger equation. Since the potential is an even function of x , one can choose the two solutions to have definite parity. The even-parity solution has the form

$$\psi_+(x) = A_+ \cos kx \quad |x| < a \quad (29a)$$

$$\psi_+(x) = \cos(k|x| + \delta_+) \quad |x| > a \quad (29b)$$

while the odd-parity one has

$$\psi_-(x) = A_- \sin kx \quad |x| < a \quad (30a)$$

$$\psi_-(x) = \epsilon(x) \sin(k|x| + \delta_-) \quad |x| > a \quad (30b)$$

where A_\pm are constants, $\epsilon(x)$ is the sign function and δ_\pm are phase shifts. A scattering solution can be written as a linear combination of ψ_\pm , so we have

$$R = \frac{1}{2}(e^{i2\delta_+} - e^{i2\delta_-}) \quad (31a)$$

$$T = \frac{1}{2}(e^{i2\delta_+} + e^{i2\delta_-}). \quad (31b)$$

The phase shifts are determined by the connection condition at $x = a$:

$$\psi(a^+) = \psi(a^-) \quad (32a)$$

$$\psi'(a^+) - \psi'(a^-) = \frac{\Omega}{a^\alpha} \psi(a). \quad (32b)$$

The result is

$$\tan \delta_+ = \frac{b \cos^2 \xi}{-\xi^\alpha + b \sin \xi \cos \xi} \quad (33a)$$

$$\tan \delta_- = -\frac{b \sin^2 \xi}{\xi^\alpha + b \sin \xi \cos \xi} \quad (33b)$$

where $\xi = ka$ and $b = \Omega k^{\alpha-1}$. Then we consider the limit $a \rightarrow 0$ (or $\xi \rightarrow 0$). If $\alpha = 0$, we have $\tan \delta_+ = -b = -\Omega/k$ and $\tan \delta_- = 0$. This leads to the known result for an ordinary $\delta(x)$ potential [1]. If $\alpha < 0$, we have $\tan \delta_+ = \tan \delta_- = 0$, so $R = 0$, $T = 1$, that is, total transmission. This is an expected result since there is actually no singularity in this case. If $\alpha > 0$, we have in general $\tan \delta_+ = \infty$ and $\tan \delta_- = 0$, so $R = -1$, $T = 0$, that is, total reflection with a phase shift π (this is not referred to the above δ_\pm). This is also an expected result since the singularity is strong in this case. However, if $\alpha = 1$ and $b = -1$ (or $\Omega = -1$), we have $\tan \delta_+ = \infty$ and $\tan \delta_- = \infty$, so $R = 0$, $T = -1$, that is, total transmission with a phase shift π . This is an unexpected result since it is among the cases with strong singularity. We point out that there exists a half-bound state with zero energy and odd parity in this case (for any finite a).

As in three and two dimensions, we now consider the square well potential

$$V^a(x) = \begin{cases} \Omega \hbar^2 / 2\mu a^{\alpha+1} & |x| < a \\ 0 & |x| > a. \end{cases} \quad (34)$$

This gives the integration $\int V^a(x) dx = \Omega \hbar^2 / \mu a^\alpha$, the same as given by the double delta potential (4). Thus when $a \rightarrow 0$ they are expected to tend to the same contact potential. The phase shifts for this potential are determined by

$$\tan \delta_+ = \frac{\eta \tan \eta - \xi \tan \xi}{\xi + \eta \tan \xi \tan \eta} \quad (35a)$$

$$\tan \delta_- = \frac{\xi \tan \eta - \eta \tan \xi}{\eta + \xi \tan \xi \tan \eta} \quad (35b)$$

where ξ is defined as before, and $\eta = \sqrt{\xi^2 - b\xi^{1-\alpha}}$. Then we let $\xi \rightarrow 0$ and analyse the behaviour of the phase shifts. After careful calculations, it is found that they lead to expected results when $\alpha \neq 1$, and when $\alpha = 1$ but Ω does not take on specific values. An unexpected result is obtained when $\alpha = 1$ and Ω takes on values from one of the two sets given below. The first nontrivial result is $R = 0$, $T = -1$, i.e. total transmission with a phase shift π . This is the same as for the double delta potential, but it happens when

$$\Omega = -\frac{(2N-1)^2\pi^2}{4} \quad (36)$$

where N is a natural number, which is different from the previous value. Note that there exists a half-bound state with odd parity (for $\alpha = 1$ and finite a) when Ω takes on any one of the above values. In contrast, for the double delta potential such a state can appear only once when $\Omega = -1$. The second nontrivial result is $R = 0$, $T = 1$, i.e. true total transmission. This happens when

$$\Omega = -N^2\pi^2 \quad (37)$$

where N is a natural number. There is no similar result for the double delta potential. Note that there exists a half-bound state with even parity for the square well potential when Ω takes on values from this sequence, while for the double delta potential there exists no such state. Thus we see once again that the difference in the unexpected result is related to the different situation for the appearance of half-bound states.

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