

USE OF SCATTERING AMPLITUDE TO RECONSTRUCT THE POTENTIAL NEAR ITS BOUNDARY

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The "asymptotic Born approximation" is formulated from the scattering amplitude for a potential that coincides with the true potential at sufficiently large radii. The order of magnitude of the relative error in the determination of the scattering potential at a point

r is $\int_r^{\infty} U(r') r' dr'$. The case where the scattering amplitude is given in a finite energy

interval is considered.

INTRODUCTION

THE methods presented in the literature for solving the problem of potential reconstruction use, as data on scattering, the phase corresponding to one of the values of the orbital momentum.¹⁻³ An exception is the work of Moses,⁴ who uses the amplitude of the backward scattering. The use of the scattering amplitude instead of the phase is more logical, first because it may, in principle, be determined from the scattering cross section without a phase analysis,⁵ and second because the use of the scattering amplitude makes it possible to consider arbitrary and not only spherically symmetric potentials.

In the case of an arbitrary potential, the scattering amplitude depends on five values: the energy and the components of two unit vectors, in the directions of the initial and final momenta. The potential depends only on three components of the radius vector. The resulting indeterminacy of the inverse problem is easiest to eliminate for weak potentials: in that case, the scattering amplitude depends, in first approximation, only on the vector of momentum transfer, i.e., on three parameters. A simple Fourier transformation is then sufficient to reconstruct the potential simultaneously in the whole space. For strong potentials, the first Born approximation for the scattering amplitude is correct only for large energies and for not very small vectors of momentum transfer. This means that, in the case of strong potentials, the first Born approximation for the potential is meaningless.

In the present paper we shall construct an "asymptotic Born approximation" for a potential having the following properties: in the case of

weak potentials, it coincides with the usual first approximation and yields the real potential simultaneously in the whole space. As the potential increases, the accuracy of the approximation decreases, but not uniformly; it decreases faster near the central regions and slower near the potential boundary. (Only potentials lying wholly in a certain finite region of the space are considered.) Thus, the "asymptotic approximation" for a potential of any value will correctly reconstruct its behavior in a certain layer near the boundary; the thickness of the layer is determined by the value of the potential.

The simplicity of constructing the "asymptotic approximation" makes it easily possible to assess errors introduced by the finiteness of the energy interval in which the scattering amplitude is given. Thus, in the framework of this approximation, one can disregard the academic problem of determining the potential from data at all energies from zero to infinity, and approach the solution of the practical problem formulated by Smorodinskii,⁶ that of reconstructing the potential from a scattering amplitude given in a finite energy interval. The over-determination of the problem is also removed in this approximation. It is found that, in order to construct the "asymptotic approximation," only the dependence of the scattering amplitude on the momentum transfer vector is essential.

All proofs use the representation of the scattering amplitude by a Born approximation series (the derivation of which can be seen for instance, in the paper by Moses,⁴ Sec. 5). The one-dimensional Fourier transformation of this series for fixed directions of the incident and scattering particle was used by Wong⁷ to obtain the dispersion relations in the nonrelativistic case. In the same

paper, a method of determining the potential boundary from the scattering amplitude is given.

Strictly speaking, all assumptions of the present paper are correct only for potentials for which the Born approximation series converges uniformly for all energies. However, the character of the results makes it possible to assume that the use of these series is only a subsidiary means, which makes the proof simpler, but the basic result is correct also for potentials for which the Born approximation series for the scattering amplitude is divergent.

1. FOURIER TRANSFORMATION

The scattering amplitude is a function of the wave number k and the two unit vectors \mathbf{n}_1 and \mathbf{n}_2 in the direction of the initial and final momentum of the particle, defined only for positive values of k . It will be convenient, however, to consider a definition extended to the negative values of k by means of the equation

$$f(\mathbf{n}_2, k, \mathbf{n}_1) = f^*(\mathbf{n}_2, |k|, \mathbf{n}_1), \quad k < 0. \quad (1)$$

We shall introduce new variables \mathbf{n} and \mathbf{N} :

$$\mathbf{n} = \mathbf{n}_2 - \mathbf{n}_1, \quad n \leq 2, \quad (2)$$

$$\mathbf{N} = (\mathbf{n}_2 + \mathbf{n}_1) / 2, \quad N \leq 1, \quad (3)$$

and the momentum transfer vector \mathbf{q} :

$$\mathbf{q} = k \mathbf{n}_2 - k \mathbf{n}_1 = k \mathbf{n}, \quad \mathbf{q}_0 = \mathbf{q} / q, \quad (4)$$

The vectors \mathbf{n} and \mathbf{N} are orthogonal and their absolute values are determined by the polar scattering angle ϑ :

$$\cos \vartheta = (\mathbf{n}_2, \mathbf{n}_1), \quad n = 2 \sin(\vartheta / 2), \quad N = \cos(\vartheta / 2). \quad (5)$$

The scattering amplitude can also be considered as a function of the new variables q , \mathbf{q}_0 , and \mathbf{N} where, according to Eq. (1), the value q takes all possible values $-\infty < q < \infty$.

We shall fix the direction of the initial and final momenta or, which is the same, of the vectors \mathbf{q}_0 and \mathbf{N} , and we shall perform the following Fourier transformation:

$$F(\rho, \mathbf{q}_0, \mathbf{N}) = 2 \int_{-\infty}^{\infty} f(q, \mathbf{q}_0, \mathbf{N}) \exp(iq\rho) dq \equiv 2 \int_{-\infty}^{\infty} f(\mathbf{n}_2, k, \mathbf{n}_1) \exp(ikn\rho) d(kn). \quad (6)$$

The function F may be written as a series

$$F(\rho, \mathbf{q}_0, \mathbf{N}) = (4\pi)^{-1} \sum_{l=1}^{\infty} (-1)^l U_l(\rho, \mathbf{q}_0, \mathbf{N}), \quad (7)$$

the terms of which are determined by the scatter-

ing potential $U(r)$, and which represent the Fourier transformations of the terms of the Born approximation series

$$U_l(\rho, \mathbf{q}_0, \mathbf{N}) = 2 \int_{-\infty}^{\infty} B_l(\mathbf{n}_2, k, \mathbf{n}_1) \exp(ikn\rho) n dk. \quad (8)$$

Because of the exponential dependence of B_l on k , after integrating over dk in the expression for U_l , the one-dimensional δ -function appears under the sign of integration over the coordinates:

$$U_1(\rho, \mathbf{q}_0) = \int U(\mathbf{r}) \delta(-\mathbf{q}_0 \mathbf{r} + \rho) d\mathbf{r}, \quad (9)$$

$$U_l(\rho, \mathbf{q}_0, \mathbf{N}) = (4\pi)^{-l+1} \times \int \frac{U(\mathbf{x}) U(\mathbf{z}_1) \dots U(\mathbf{z}_{l-2}) U(\mathbf{y})}{|\mathbf{x} - \mathbf{z}_1| \dots |\mathbf{z}_{l-2} - \mathbf{y}|} \delta(-\mathbf{n}_2 \mathbf{x} + |\mathbf{x} - \mathbf{z}_1| + \dots + |\mathbf{z}_{l-2} - \mathbf{y}| + \mathbf{n}_1 \mathbf{y} + n\rho) n dk \dots d\mathbf{y}. \quad (10)$$

Setting the arguments of the δ -function equal to zero, we obtain equations that determine the range of integration over the coordinates.

The first term is especially simple

$$U_1(\rho, \mathbf{q}_0) = \int_{r_{\mathbf{q}_0} = \rho} U(\mathbf{r}) dS, \quad (11)$$

and reduces to a double integral of the potential in the plane determined by the following equation:

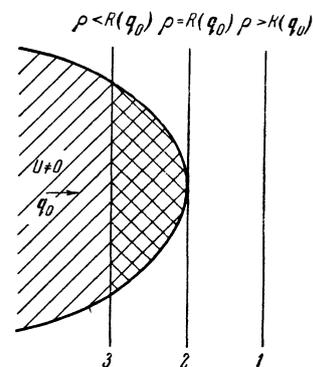
$$r_{\mathbf{q}_0} = \rho. \quad (12)$$

This plane is perpendicular to the vector \mathbf{q}_0 , and its distance from the point of origin of the coordinates is equal to ρ if we consider the direction of \mathbf{q}_0 as positive.

The remaining terms are analyzed in detail in the Appendix, where it is shown that the integration over all variables is carried out only in that part of the space where

$$r_{\mathbf{q}_0} \geq \rho. \quad (13)$$

The first conclusion we can draw is that if the plane (12) lies beyond the potential boundaries (see figure, straight line 1), then the transforma-



tion (6) of the scattering amplitude equals zero:

$$F(\rho, \mathbf{q}_0, \mathbf{N}) \equiv 0, \quad \rho \geq R(\mathbf{q}_0). \quad (14)$$

The radius of the potential in the direction $\mathbf{q}_0 R(\mathbf{q}_0)$ is equal to that value of ρ for which the plane (12) is tangent to the potential boundary (straight line 2 in the figure). Equation (13) was first obtained by Wong.⁷

In the Appendix it is also shown that, for $\rho < R(\mathbf{q}_0)$, the value of the first term in the series (7) and the sum of the other terms can be estimated in the following way:

$$\begin{aligned} |U_1(\rho, \mathbf{q}_0)| &\approx \bar{U} \bar{r}^2, & (15) \\ \left| \sum_{l=r}^{\infty} U_l \right| &\approx (\bar{U} \bar{r}^2) (\bar{\Delta}^2), & (16) \end{aligned}$$

where \bar{r} represents the mean linear dimensions of the area cut in the region $U \neq 0$ by the plane (12). These estimates are basically correct only for small values of the difference Δ :

$$\Delta = R(\mathbf{q}_0) - \rho. \quad (17)$$

The value of $\bar{\Delta}$ in Eq. (16) is equal to the smallest of the numbers \bar{r}, Δ

$$\bar{\Delta} = \min\{\bar{r}, \Delta\}. \quad (18)$$

From the estimates (15) and (16), it follows that in the equation

$$F(\rho, \mathbf{q}_0, \mathbf{N}) = U_1(\rho, \mathbf{q}_0) [1 + \varepsilon(\rho, \mathbf{q}_0, \mathbf{N})] \quad (19)$$

the value of ε for sufficiently small Δ is determined by the following approximate relations

$$\begin{aligned} |\varepsilon(\rho, \mathbf{q}_0, \mathbf{N})| &\approx \bar{U} \bar{\Delta}^2 \ll \bar{U} \bar{r}^2 \\ &\approx |U_1(\rho, \mathbf{q}_0)| \approx |F(\rho, \mathbf{q}_0, \mathbf{N})|. \end{aligned} \quad (20)$$

We summarize the results of this section: Let the scattering amplitude be given in such a way that the vector \mathbf{q}_0 assumes all possible directions and the length of the momentum-transfer vector goes through all possible values from zero to infinity for each direction of \mathbf{q}_0 . In such a case, the scattering amplitude permits us to construct a function $F(\rho, \mathbf{q}_0, \mathbf{N})$ for all values of ρ and directions \mathbf{q}_0 . According to Eq. (14), this function is identically equal to zero for sufficiently large values of ρ . The largest value of ρ for which F is different from zero determines the potential boundary in the direction \mathbf{q}_0 , namely the value $R(\mathbf{q}_0)$. It is evident that the envelope of all tangential planes obtained in such a way determines the exact potential boundary. For values of ρ smaller than $R(\mathbf{q}_0)$ but sufficiently close to it, and where the value of Δ is small, the following approximate equation is correct:

$$F(\rho, \mathbf{q}_0, \mathbf{N}) \approx U_1(\rho, \mathbf{q}_0), \quad (21)$$

which determines the integral of the potential in the plane (12). The relative error of Eq. (21) is equal to the absolute value of the function F , i.e., the integrals of the potential in planes cutting its external layers are determined very accurately, but only rather roughly in planes which encompass the central regions.

We shall note that, for a centrally symmetric potential, the value $U_1(\rho, \mathbf{q}_0)$ is given by the integral

$$U_1(\rho, \mathbf{q}_0) = 2\pi \int_{\rho}^{\infty} U(r) r dr, \quad (22)$$

which determines the accuracy of Eq. (21).

It is interesting to obtain equations which determine the potential of $U(\mathbf{r})$ itself rather than integrals of it. It will be shown below that Eq. (21) makes it possible to construct a certain approximate potential F which has the same boundary as the true scattering potential and coincides with the boundary with an accuracy given by Eq. (20).

2. THE ASYMPTOTIC BORN APPROXIMATION

We shall make use of the approximate expression (21) for the inverse transition from the function U_1 to the potential $U(\mathbf{r})$. If the function $U_1(\rho, \mathbf{q}_0)$ were known accurately, then, for a single-valued reconstruction of the potential, it would be sufficient to perform two Fourier transformations on it:

$$U(\mathbf{q}) = \int U_1(\rho, \mathbf{q}_0) \exp(-iq\rho) d\rho, \quad q > 0 \quad (23)$$

and

$$U(\mathbf{r}) = (2\pi)^{-3} \int U(\mathbf{q}) \exp(i\mathbf{q}\mathbf{r}) d\mathbf{q}. \quad (24)$$

It can easily be seen that the function $F(\rho, \mathbf{q}_0, \mathbf{N})$ is not a transformation of the type $U_1(\rho, \mathbf{q}_0)$ of any fictitious potential and, consequently, it is impossible to apply transformations (23) and (24) to it directly. In fact, were such a fictitious potential to exist, the function F would have the form of a double integral

$$F(\rho, \mathbf{q}_0, \mathbf{N}) = \int_{r_{\mathbf{q}_0}=\rho} F(\mathbf{r}) dS, \quad (25)$$

and would therefore satisfy the condition

$$F(\rho, \mathbf{q}_0, \mathbf{N}) = F(-\rho, -\mathbf{q}_0, \mathbf{N}). \quad (26)$$

As can be seen from Eq. (13), which determines the region of integration, $F(\rho, \mathbf{q}_0, \mathbf{N})$ depends on the behavior of the potential in the region $r_{\mathbf{q}_0} \geq \rho$, and $F(-\rho, -\mathbf{q}_0, \mathbf{N})$ depends on the behavior of the potential when $r_{\mathbf{q}_0} \leq \rho$, so that condition (26) cannot be

satisfied. However, it is clear from these considerations how to circumvent this difficulty. To this end, we introduce a new function F by means of the two equations

$$F(\rho, \mathbf{q}_0, \mathbf{N}) = \begin{cases} F(\rho, \mathbf{q}_0, \mathbf{N}), & \rho > 0, \\ F(-\rho, -\mathbf{q}_0, \mathbf{N}) & \rho < 0. \end{cases} \quad (27)$$

A certain approximate potential $F(\mathbf{r}, \mathbf{N})$ corresponds to the new function. To obtain a three-dimensional Fourier component of this potential, we substitute Eq. (27) in Eq. (23) and make use of the definition (6) of the function F . We have

$$f^+(\mathbf{q}, \mathbf{N}) \equiv \int F(\rho, \mathbf{q}_0, \mathbf{N}) \exp(-i\rho\mathbf{q}) d\rho = \int [f(q', \mathbf{q}_0, \mathbf{N}) \times \delta_+(q' - q) + f^*(q', -\mathbf{q}_0, \mathbf{N}) \delta_+(q - q')] dq'. \quad (28)$$

The final result can be formulated in the following manner: If the scattering amplitude is transformed according to Eq. (28), and we then use the transformed amplitude for constructing the first Born approximation for the potential, then the approximation obtained will have exactly the same boundary as the true potential and will coincide with it near the boundary with an accuracy of order of magnitude equal to the product

$$\overline{U(\mathbf{r})} \Delta^2(\mathbf{r}),$$

where Δ is the shortest distance from the point at which the potential is determined to the boundary, and \overline{U} is the average value of the potential between the point \mathbf{r} and the boundary.

Let us return to the experimental data necessary for reconstructing the potential. It is clear that the unit vector \mathbf{q}_0 does not determine the scattering amplitude in a unique way: there still remains an ambiguity in the choice of the vector \mathbf{N} . According to Eq. (19) – (21), for any choice of the vector \mathbf{N} , the reconstructed potential will coincide with the true one in a single layer near the boundary with the same accuracy. This means that not only the potential is obtained, but also the condition which should be satisfied by the scattering amplitude of any potential. The transformed scattering amplitude determines a fictitious potential $F(\mathbf{r}, \mathbf{N})$, the value of which is independent of the vector \mathbf{N} within the limits of the error (20).

In any practical case, the scattering amplitude will be given only up to a certain finite value of q_{\max} . It is evident that the replacing of the infinite range of integration by a finite one leads to the averaging of the approximate potential $F(\mathbf{r})$ over a certain volume, the linear dimensions l of which are determined by the value q_{\max} :

$$lq_{\max} \approx \pi. \quad (29)$$

If it is necessary that the relative error in the determination of the potential be smaller than ϵ , then the value of l should satisfy the condition

$$l \leq \Delta, \quad (30)$$

where $\Delta = \Delta(\epsilon)$ is determined by the condition that, in a layer at the depth Δ near the boundary, the approximate potential $F(\mathbf{r})$ is equal to the true potential $U(\mathbf{r})$ with the relative error not bigger than ϵ . This condition is satisfied if

$$\overline{U} \Delta^2 \leq \epsilon. \quad (31)$$

From Eqs. (29), (30), and (31), and substituting for q_{\max} the maximum energy up to which the scattering amplitude is known,

$$E_{\max} = k_{\max}^2 = q_{\max}^2 [2 \sin(\vartheta/2)]^{-2}, \quad (32)$$

we obtain a new inequality

$$E_{\max} \geq (\pi^2/4) |\overline{U}| \varepsilon^{-1} \sin^{-2}(\vartheta/2). \quad (33)$$

From this inequality it follows that, in practice, it is more convenient to use the backward scattering amplitude, in which case it is necessary to measure it in a minimum energy interval.

Thus, for instance, for a rough determination of the order of magnitude, for the case where $\epsilon \approx 1$, the backward scattering amplitude should be measured to the value

$$E_{\max} > 2 |\overline{U}(\mathbf{r})| \quad (34)$$

and, to the contrary, if the scattering amplitude at an angle π is known up to the energy E_{\max} , then, on this basis, it is impossible, to reconstruct the potential in that region even roughly, if its order of magnitude is bigger than or equal to E_{\max} .

CONCLUSION

All the results of the present paper are also applicable to the scattering of particles with spin, but in that case it is necessary to consider the potential in a form of a matrix and to introduce the spin function into all plane waves.

Strictly speaking, all the above results have been proven only for bounded potentials for which the Born approximation series converges for all energies. However, the series may diverge, owing to integration over the whole range where the potential is different from zero, while in the series (6) the integration extends only over the external segment of the potential. Therefore, it seems highly probable that the divergence of the series (7) is quite independent of the behavior of the potential in the deep regions, since the use of the total series of the Born approximations is simply

the most convenient method of proof.

In that case, in order that the theorems be correct it is only necessary that the transformation $U_1(\rho, \mathbf{q}_0)$ tend to zero for $\rho \rightarrow \infty$, which is the case for all potentials that decrease at infinity so that $r^2U(\mathbf{r}) \rightarrow 0$ for $r \rightarrow \infty$.

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APPENDIX

The sum $-\mathbf{n}_2\mathbf{x} + \mathbf{n}_1\mathbf{y}$ expressed in terms of the variables (2) - (4) in the new coordinates \mathbf{Z} and \mathbf{z}

$$\mathbf{Z} = (\mathbf{x} + \mathbf{y}) / 2, \tag{A1}$$

$$\mathbf{z} = (\mathbf{x} - \mathbf{y}) / 2, \tag{A2}$$

can be written in the following way:

$$-\mathbf{n}_2\mathbf{x} + \mathbf{n}_1\mathbf{y} = - (n \mathbf{q}_0\mathbf{Z} + 2 N\mathbf{z}). \tag{A3}$$

The sum $|\mathbf{x} - \mathbf{z}_1| + |\mathbf{z}_1 - \mathbf{z}_2| + \dots + |\mathbf{z}_{l-2} - \mathbf{y}|$ represents the length of a broken line connecting the ends of the vectors \mathbf{x} and \mathbf{y} ; it is greater than the length of the vector $\mathbf{x} - \mathbf{y} = 2\mathbf{z}$:

$$|\mathbf{x} - \mathbf{z}_1| + \dots + |\mathbf{z}_{l-2} - \mathbf{y}| = 2z + \beta, \beta \geq 0. \tag{A4}$$

Making use of all these transformations, we shall express the vanishing of the argument of the δ -function in the l -th term of the series (7) [see Eq. (10)] in the following way:

$$n[\mathbf{q}_0\mathbf{Z} - \rho] = 2[z + N\mathbf{z}] + \beta. \tag{A5}$$

On the right-hand side we have a sum of positive values [see Eq. (3)]. Therefore the difference on the left hand side should also be positive.

$$\mathbf{q}_0\mathbf{Z} \geq \rho. \tag{A6}$$

For a fixed \mathbf{Z} and β , the projection of the vector \mathbf{z} on the direction \mathbf{q}_0 may be expressed as a function of the angle α between the vectors \mathbf{N} and \mathbf{z} :

$$|\mathbf{q}_0\mathbf{z}| = \sin \alpha [n(\mathbf{q}_0\mathbf{Z} - \rho) - \beta] / [2(1 - N \cos \alpha)]. \tag{A7}$$

In the last equation, we make use of the orthogonality of the vectors \mathbf{q}_0 and \mathbf{N} . This function has a maximum if $\cos \alpha = N$. Making use of expressions (5) for N and n , we obtain for the maximum value of this projection

$$|\mathbf{q}_0, \mathbf{z}|_{max} = \mathbf{q}_0\mathbf{Z} - \rho, \tag{A8}$$

from which follows the required limitation of the integration region over variables \mathbf{x} and \mathbf{y} :

$$x\mathbf{q}_0 \geq \rho, \quad y\mathbf{q}_0 \geq \rho. \tag{A9}$$

The variables \mathbf{z}_i remain to be considered. It

is clear that any of the vertices of the broken line $2z + \beta$ cannot deviate from the end of vector \mathbf{Z} in the direction \mathbf{q}_0 by more than $z + \beta/2$, while the maximum deviation is attained when the directions of the vectors \mathbf{q}_0 and \mathbf{z} coincide; in that case $\mathbf{zN} = 0$. The last equation makes it possible to estimate the sum $z + \beta/2$ from Eq. (A6)

$$z + \beta/2 = \sin(\vartheta/2) [\mathbf{q}_0\mathbf{Z} - \rho]. \tag{A10}$$

Whence follows the proof:

$$z_i\mathbf{q} \geq \rho. \tag{A11}$$

Thus, the range of integration over the variables \mathbf{x} and \mathbf{y} extends over the crosshatched segment. The contribution of the integral over these variables to the total integral U_l can be estimated as the product

$$(\bar{U} \bar{r}^2) (\bar{U} \Delta^2). \tag{A12}$$

For fixed vectors \mathbf{x} and \mathbf{y} , the vectors \mathbf{z}_i all lie in a sphere of radius

$$\sin(\vartheta/2) [\mathbf{q}_0\mathbf{Z} - \rho],$$

with its center at \mathbf{Z} , and therefore the integral over these variables contains no \bar{r} but a certain $\bar{\Delta}$ equal to the smallest of the numbers \bar{r}, Δ .

The total integral U_l can be estimated in the following way:

$$|U_l| \approx (\bar{U} \bar{r}^2) (\bar{U} \Delta^2)^{l-1} \tag{A13}$$

If the expressions obtained are summed up over l from $l = 2$ to ∞ , we obtain the following estimate for the sum of all terms of the series (7) without the first one:

$$\left| \sum_{l=2}^{\infty} U_l \right| \approx (\bar{U} \bar{r}^2) (\bar{U} \Delta^2) / [1 - (\bar{U} \Delta^2)]. \tag{A14}$$

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