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Exactly solvable three-dimensional scattering problem

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Schrödinger's equation is solved exactly for a potential vanishing outside a prolate spheroid. The potential is then reconstructed from the first Born approximation for the scattering amplitude.

I. INTRODUCTION

Exactly solvable examples of quantum-mechanical scattering problems are well known and described in most texts on quantum mechanics. However, invariably, such examples refer either to one-dimensional problems or to cases with spherical symmetry. Nontrivial examples which are neither one dimensional nor with spherical symmetry are harder to come by, particularly if they are not to be mathematically too elaborate. Presenting such an example is the purpose of this article. It involves a potential of a special form, vanishing outside a prolate spheroid. In Sec. II, given this potential, the direct scattering problem, consisting in finding the scattering amplitude, is solved exactly. In Sec. III it is shown that the problem can also be reversed and the potential determined from the scattering amplitude; the potential reconstruction presented here will involve, though, only the Born approximation of the total amplitude.

II. DIRECT PROBLEM

Prolate spheroidal (PS) coordinates, ξ, η, ϕ, are defined through their relations to Cartesian coordinates:

$$\begin{aligned} x &= (d/2)[(\xi^2-1)(1-\eta^2)]^{1/2}\cos\phi, \\ y &= (d/2)[(\xi^2-1)(1-\eta^2)]^{1/2}\sin\phi, \\ z &= (d/2)\xi\eta, \end{aligned} \tag{2.1}$$

where $1 \leqslant \xi < \infty$, $-1 \leqslant \eta \leqslant 1$, $0 \leqslant \phi \leqslant 2\pi$. The surfaces $\xi =$ const are prolate spheroids (generated by rotating ellipses about their major axes), and d is the interfocal distance. All notations relating to PS coordinates or the solutions of the Helmholtz equation in PS coordinates are taken without exception from the monograph by Flammer.[1]

Schrödinger's equation

$$(\Delta + k^2)\phi = V\phi \tag{2.2}$$

in PS coordinates reads

$$\frac{1}{\xi^2-\eta^2}\left(\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}+\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} + \frac{\xi^2-\eta^2}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial\phi^2}\right)\phi + c^2\phi = (d/2)^2 V\phi, \tag{2.3}$$

where $c = k(d/2)$. From the class of potentials for which Eq. (2.3) is separable we choose

$$V(\xi,\eta) = \frac{\gamma^2}{(d/2)^2}\frac{\xi^2}{\xi^2-\eta^2}\theta(\xi_0-\xi), \tag{2.4}$$

where γ^2 is a positive (coupling) constant, $\xi_0 > 1$ is a fixed value of ξ, and θ is the Heaviside function. The potential (2.4) is not meant to describe any particular physical situation, even though one might think of some molecular forces it could model (note the singularities at the two foci).

The ϕ dependence of the solution is given by trigonometric funcitons $\cos m\phi$ and $\sin m\phi$, with m an integer. The other angular function and the radiatial function satisfy, respectively, the equations

$$\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta}S_{mn}(\eta) + \left(\lambda_{mn}(c) - c^2\eta^2 - \frac{m^2}{1-\eta^2}\right)S_{mn}(\eta) = 0, \tag{2.5}$$

$$\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi}R_{mn}(\xi) - \left(\lambda_{mn}(c) - [c^2-\gamma^2\theta(\xi_0-\xi)]\xi^2 + \frac{m^2}{\xi^2-1}\right)R_{mn}(\xi) = 0, \tag{2.6}$$

where λ_{mn} (m, n integers) are separation constants for which there exist extensive tabulations. Equation (2.5) has two independent solutions; the first reduces, as $c \to 0$ and $\lambda_{mn} \to n(n+1)$, to the associated Legendre function $P_n^m(\eta)$, while the second to $Q_n^m(\eta)$. The second solution is not acceptable in this context, and the first will be denoted simply by $S_{mn}(c,\eta)$.

The radial equation (2.6) also has two solutions, corresponding to the spherical Bessel functions $j_l(kr)$ and $y_l(kr)$ occurring in problems with spherical symmetry, and will be denoted by $R_{mn}^{(1)}(c,\xi)$ and $R_{mn}^{(2)}(c,\xi)$, respectively, for $1 \leqslant \xi \leqslant \xi_0$, and by $R_{mn}^{(1)}(\alpha,\xi)$ and $R_{mn}^{(2)}(\alpha,\xi)$, where

$$\alpha = (c^2-\gamma^2)^{1/2} \tag{2.17}$$

for $\xi \geqslant \xi_0$.[2] The combinations

$$\begin{aligned} R_{mn}^{(3)} &= R_{mn}^{(1)} + iR_{mn}^{(2)}, \\ R_{mn}^{(4)} &= R_{mn}^{(1)} - iR_{mn}^{(2)} \end{aligned} \tag{2.8}$$

corresponding to the spherical Hankel functions are also of interest.

The solution for $1 \leqslant \xi \leqslant \xi_0$ can be written as

$$\phi = 2\sum_{m,n}\frac{2-\delta_{0m}}{N_{mn}} i^n A_{mn} S_{mn}(c,\eta) \times R_{mn}^{(1)}(\alpha,\xi)\cos m(\phi-\phi_0), \tag{2.9}$$

with coefficients A_{mn} to be determined.

For $\xi \geqslant \xi_0$ it is convenient to separate the plane-wave contribution from that of the scattered wave:

$$\phi = e^{i\mathbf{k}\mathbf{r}} + \phi_s, \tag{2.10}$$

and, because $\eta \to \cos\theta$ and $c\xi \to kr$ as $r \to \infty$, so that

$$R_{mn}^{(3)}(c,\xi) \underset{r\to\infty}{\sim} \frac{(-i)^{n+1}}{kr}e^{ikr}, \tag{2.11}$$

ϕ_s can be written as

$$\phi_s = 2 \sum_{m,n} \frac{2-\delta_{0m}}{N_{mn}} i^n B_{mn} S_{mn}(c,\eta) \times R^{(3)}_{mn}(c,\xi)\cos m(\phi-\phi_0), \quad (2.12)$$

again with coefficients B_{mn} to be determined. In Eqs. (2.9) and (2.12), $N_{mn}(c)$ are normalization constants for the angular functions which satisfy the orthogonality relations:

$$\int_{-1}^{1} S_{mn}(c,\eta) S_{mn'}(c,\eta) d\eta = N_{mn}(c)\delta_{nn'}. \quad (2.13)$$

Following the standard procedure, one expands the plane wave in PS coordinates,

$$e^{i\mathbf{k}\mathbf{r}} = 2\sum_{m,n}\frac{2-\delta_{0m}}{N_{mn}} i^n S_{mn}(c,\cos\theta_0) \times S_{mn}(c,\cos\theta) R^{(1)}_{mn}(c,\xi)\cos m(\phi-\phi_0), \quad (2.14)$$

and then matches the solutions (2.9) and (2.10) at $\xi=\xi_0$. One then obtains

$$A_{mn} = [R^{(1)}_{mn}(c,\xi_0) + a_{mn} R^{(3)}_{mn}(c,\xi_0)] \times R^{(1)-1}_{mn}(\alpha,\xi_0) S_{mn}(c,\cos\theta_0) \quad (2.15)$$

and

$$B_{mn} = a_{mn} S_{mn}(c,\cos\theta_0), \quad (2.16)$$

where

$$a_{mn} = -\frac{R^{(1)}_{mn}(c,\xi_0)R^{(1)\prime}_{mn}(\alpha,\xi_0) - R^{(1)\prime}_{mn}(c,\xi_0)R^{(1)}_{mn}(\alpha,\xi_0)}{R^{(3)}_{mn}(c,\xi_0)R^{(1)\prime}_{mn}(\alpha,\xi_0) - R^{(3)\prime}_{mn}(c,\xi_0)R^{(1)}_{mn}(\alpha,\xi_0)}. \quad (2.17)$$

The scattering amplitude identified in the asymptotic expression of ϕ_s, viz.,

$$\phi_s \underset{r\to\infty}{\sim} A_k(\mathbf{u}_0,\mathbf{u})\frac{e^{ikr}}{r} \quad (2.18)$$

is

$$A_k(\mathbf{u}_0,\mathbf{u}) = \frac{2}{ik}\sum_{m,n}\frac{2-\delta_{0m}}{N_{mn}} a_{mn} S_{mn}(c,\cos\theta_0) \times S_{mn}(c,\cos\theta)\cos m(\phi-\phi_0). \quad (2.19)$$

Introduction of the phase shifts $\bar{\delta}_{mn}(k)$ through the relations

$$\tan\bar{\delta}_{mn}(k) = -\mathrm{Re}\, a_{mn}/\mathrm{Im}\, a_{mn} \quad (2.20)$$

yields A_k in the form

$$A_k(\mathbf{u}_0,\mathbf{u}) = \frac{2}{k}\sum_{m,n}\frac{2-\delta_{0m}}{N_{mn}}\exp[i\bar{\delta}_{mn}(k)]\sin\bar{\delta}_{mn}(k) \times S_{mn}(c,\cos\theta_0)S_{mn}(c,\cos\theta)\cos m(\phi-\phi_0), \quad (2.21)$$

which generalizes the well-known expansion of the scattering amplitude in the case of spherical symmetry. While this expansion has been obtained here for a special potential, it is clear that its form remains the same in general, for any potential vanishing fast enough as $\xi\to\infty$. It is therefore evident that while $A_k(\mathbf{u}_0,\mathbf{u})$ is indeed a function of five variables, it is in effect determined by a function of only three variables (two discrete, m and n, and one continuous, k): $\bar{\delta}_{mn}(k)$, whereas the potential (2.4) depends on only two variables. This circumstance is to be compared with the situation in the spherically symmetric case, where the potential is a function of one variable, but the scattering amplitude, through the phase shifts $\delta_l(k)$, is determined by a function of two variables (one discrete, l, and one continuous, k).

III. INVERSE PROBLEM

We propose now to show how the potential can be reconstructed from the scattering amplitude. The solution to this inverse scattering problem for one-dimensional or spherically symmetric cases has been known for some time and is described in detail in some excellent texts.[3] The solution in the general three-dimensional case has only recently been worked out by Newton,[4] and the main steps to be followed will be briefly described below.

Namely, as Newton shows, the potential $V(\mathbf{r})$ can be reconstructed, in the absence of bound states, from the formula

$$V(\mathbf{r}) = -2\mathbf{u}_0\cdot\nabla K(\mathbf{u}_0,\mathbf{u}_0\cdot\mathbf{r},\mathbf{r}), \quad (3.1)$$

where $\mathbf{u}_0$ is the unit vector of the direction of propagation of the incoming plane wave [$\exp(i\mathbf{k}\mathbf{r})$, $\mathbf{k}=k\mathbf{u}_0$], and K is the solution of a generalized Marchenko equation:

$$K(\mathbf{u}_0,s,\mathbf{r}) = \int d^2\mathbf{u}\Big(G(\mathbf{u}_0,\mathbf{u},s+\mathbf{u}\cdot\mathbf{r}) + \int_{\mathbf{u}\cdot\mathbf{r}}^{\infty} dt\, G(\mathbf{u}_0,\mathbf{u},s+t)K(\mathbf{u},t,\mathbf{r})\Big), \quad (3.2)$$

where $d^2\mathbf{u}$ indicates two-dimensional integration over the direction of the unit vector $\mathbf{u}$($d^2\mathbf{u}=\sin\theta\, d\theta\, d\phi$). The input function G is given in terms of the scattering amplitude $A_k(\mathbf{u},\mathbf{u}_0)$:

$$G(\mathbf{u}_0,\mathbf{u},s) = \left(\frac{i}{4\pi^2}\right)\int_{-\infty}^{\infty} dk\, kA_k(-\mathbf{u}_0,\mathbf{u})e^{-iks}. \quad (3.3)$$

The solution (3.1) requires, therefore, knowledge of the scattering amplitude for all k and all directions of the incoming plane wave $\mathbf{u}_0$, as well as for all directions of the outgoing spherical wave $\mathbf{u}$.

This procedure can be significantly simplified in the present case, due to the fact that the scattering amplitude is available here as a (Born) expansion in powers of γ^2. Indeed in this case the function G of (3.3) is also available as a series in powers of γ^2, and so is $K(\mathbf{u}_0,s,\mathbf{r})$ if one seeks it as such in solving Eq. (3.2). But, because the potential is linear in γ^2, only the first Born approximation can contribute to Eq. (3.1). In other words, as one sets $s=\mathbf{u}_0\cdot\mathbf{r}$ in the Born series of $K(\mathbf{u}_0,s,\mathbf{r})$, all terms, except the first, must vanish. That this vanishing actually happens has been checked in the case of a spherically symmetric exactly solvable problem.[5] Clearly, the Born expansion of the scattering amplitude is not generally available in inverse problems. In this theoretical case though, there is no problem in recasting the series (2.19) as a series in powers of γ^2 and then recognize that only its first term contributes to Eq. (3.1):

$$V(\mathbf{r}) = \frac{i}{2\pi^2}\mathbf{u}_0\cdot\nabla\int_{-\infty}^{\infty} dk\, k\, d^2\mathbf{u}\, A_k^{*(1)}(-\mathbf{u}_0,\mathbf{u}) \times\exp[ik(\mathbf{u}+\mathbf{u}_0)\cdot\mathbf{r}], \quad (3.4)$$

where $A_k^{(1)}$ is the first Born approximation to the scattering amplitude. This approximation can be easily retrieved from the exact result (2.19) by noting first that, because of Eq. (2.6), the numerator of a_{mn} in Eq. (2.17) can be written as

$$R_{mn}^{(1)}(c,\xi_0)R_{mn}^{(1)'}(\alpha,\xi_0)-R_{mn}^{(1)'}(c,\xi_0)R_{mn}^{(1)}(\alpha,\xi_0)$$
$$=\frac{\gamma^2}{\xi_0^2-1}\int_1^{\xi_0}d\xi'\xi'^2R_{mn}^{(1)}(c,\xi')R_{mn}^{(1)}(\alpha,\xi'). \qquad (3.5)$$

If Eq. (3.2) is substituted in Eq. (2.19), all one needs to do to obtain the first Born approximation is to set $\alpha=c$ everywhere in that expression. In this case the denominator of a_{mn} in (2.17) becomes the Wronskian

$$W[R_{mn}^{(3)}(c,\xi_0),R_{mn}^{(1)}(c,\xi_0)]=1/i(\xi_0^2-1)c. \qquad (3.6)$$

Hence,

$$A_k^{(1)}(\mathbf{u}_0,\mathbf{u})=-\gamma^2d\sum_{m,n}\frac{2-\delta_{0m}}{N_{mn}}\int_1^{\xi_0}d\xi'\xi'^2R_{mn}^{(1)2}(c,\xi')$$
$$\times S_{mn}(c,\cos\theta_0)S_{mn}(c,\cos\theta)\cos m(\phi-\phi_0). \qquad (3.7)$$

It remains now to substitute Eq. (3.7) in Eq. (3.4) and carry out the integrations. This procedure is easier than it might seem because one can give Eq. (3.4) a simple, compact form. Namely, by using Eqs. (2.13) and (2.14), one can write

$$R_{mn}^{(1)}(c,\xi')S_{mn}(c,\cos\theta_0)\cos m(\phi-\phi_0)$$
$$=\frac{(-i)^n}{4\pi}\int\exp(ik\mathbf{u}_0\mathbf{r}')S_{mn}(c,\cos\theta')$$
$$\times\cos m(\phi-\phi')d^2\mathbf{u}, \qquad (3.8)$$

where $\mathbf{r}'$ is the vector to the point of PS coordinates ξ', $\cos\theta'$, ϕ'. Substituting Eq. (3.8) in Eq. (3.7), and using Eq. (2.14) once more yields

$$A_k^{(1)}(\mathbf{u}_0,\mathbf{u})=-\gamma^2\frac{d}{8\pi}\int_1^{\xi_0}d\xi'\xi'^2$$
$$\times\int d^2\mathbf{u}'\exp[ik(\mathbf{u}_0-\mathbf{u})\mathbf{r}']. \qquad (3.9)$$

Noting now that $A_k^{(1)}$ is a real, even function of k, upon substitution of Eq. (3.9) in Eq. (3.4) one obtains

$$V(\mathbf{r})=\gamma^2\frac{(d/2)}{(2\pi)^2}\int_1^{\xi_0}d\xi'\xi'^2\int d^2\mathbf{u}'$$
$$\times\int d^3\mathbf{k}\exp[-i(\mathbf{k}_0+\mathbf{k})\mathbf{r}'](1+\mathbf{u}\cdot\mathbf{u}_0)$$
$$\times\{\exp[i(\mathbf{k}_0+\mathbf{k})\mathbf{r}]+\exp[-i(\mathbf{k}_0+\mathbf{k})\mathbf{r}]\}, \qquad (3.10)$$

where $\mathbf{k}=k\mathbf{u}$ and $\mathbf{k}_0=k\mathbf{u}_0$.

The required integrations are now elementary. First, notice that the scalar product $\mathbf{u}\cdot\mathbf{u}_0$ does not contribute: the angular part of the $\mathbf{k}$ integration averages it to zero. Second, a translation $\mathbf{k}\rightarrow\mathbf{k}-\mathbf{k}_0$ disposes of the remaining $\mathbf{u}_0$ dependence. The $\mathbf{k}$ integration can now be carried out and yields two three-dimensional Dirac functions, one of which contributes nothing to the remaining integrals. The other can be written in PS coordinates as

$$\delta(\mathbf{r}-\mathbf{r}')=[(d/2)^3(\xi^2-\eta^2)]^{-1}\delta(\xi-\xi')$$
$$\times\delta(\eta-\cos\theta')\delta(\phi-\phi'), \qquad (3.11)$$

and one finally obtains

$$V(\mathbf{r})=\frac{\gamma^2}{(d/2)^2}\frac{\xi^2}{\xi^2-\eta^2}\theta(\xi_0-\xi), \qquad (3.12)$$

which is the potential we started with in the first place.

IV. FINAL REMARKS

The potential for which the exact scattering problem has been solved here is only one of many that could be treated by considering expressions for which Schrödinger's equation can be separated. One such potential, for which the procedure would closely follow the one outlined here would be a potential vanishing outside an oblate spheroid, and for which Schrödinger's equation in oblate spheroidal coordinates is separable. Of more interest could perhaps be a potential leading to a scattering amplitude for which the integral (3.3) can be done, and the integral equation (3.2) solved, without recourse to an expansion in powers of the coupling constant.

ACKNOWLEDGMENT

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[1]C. Flammer, *Spheroidal Wave Functions* (Stanford University, Palo Alto, CA, 1957).

[2]A word of caution about this notation is in order. While it is true that $R_{mn}^{(i)}(\alpha,\xi)$ reduces to $R_{mn}^{(i)}(c,\xi)$, as defined in Ref. 3, if one sets $\alpha=c$, it is not true that $R_{mn}^{(i)}(\alpha,\xi)$ can be obtained from $R_{mn}^{(i)}(c,\xi)$ by setting $c=\alpha$, as the notation seems to suggest. To obtain explicit expressions for $R_{mn}^{(i)}(\alpha,\xi)$, one needs to retrace the procedure outlined in Ref. 3, which is straightforward but not immediate.

[3]R. G. Newton, *Scattering of Waves and Particles* (McGraw-Hill, New York, 1966), K. Chadan and P. C. Sabatier, *Inverse Problems in Quantum Scattering Theory* (Springer-Verlag, New York, 1977).

[4]R. G. Newton, Phys. Rev. Lett. **43**, 541 (1979); J. Math. Phys. **21**, 493 (1980); **21**, 1698 (1980); **22**, 631 (1981); **22**, 2191 (1981).

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