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Modification of the Newton Method for the Inverse-Scattering Problem at Fixed Energy

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The method of Newton for the solution of the inverse-scattering problem is modified with the assumption that the potential is known for radial distances $r > r_0$. The modified method is improved by applying a least-squares method.

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The inverse-scattering problem (ISP) in quantum mechanics for a spherical potential and fixed energy was first solved more generally by Newton on the basis of an analog of the Gel'fand-Levitan equation.[1,2] The Newton (Newton-Sabatier) method was extensively investigated and extended by Sabatier and co-workers,[3] who studied the nonuniqueness of the ISP and tested the procedure in numerical calculations.[3,4] These calculations were recently improved by Coudray.[5] Also different methods for the solution of the ISP at fixed energy have been applied in the framework of the WKB method[6] and for the case in which the S matrix is expanded in Regge poles and zeros.[7]

In this Letter we suggest a modification of Newton's method. We assume that the spherical potential is known from a certain radial distance r_0 up to infinity. This assumption is not stringent for most physical applications. On this basis we reformulated the equations for the coefficients, which depend on the phases, by deriving them at finite values $r > r_0$, rather than in the asymptotic region as done by Newton. This modification has the advantage that the phases determine the potential in the finite interval $(0, r_0)$ and not in the infinite interval $(0, \infty)$, as in Newton's method. Therefore, the information about the potential, given by the phases, is fully used to reproduce the potential in the physically interesting interaction region $(0, r_0)$.

Inverse scattering problem at fixed energy. —To review Newton's method[1-3] let us define the notations starting with the radial Schrödinger equation:

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r) - E\right)R_l(r) = 0. \quad (1)$$

This equation can be rewritten in the following form by use of dimensionless coordinates:

$$D_\rho{}^U \varphi_l{}^U(\rho) = l(l+1)\varphi_l{}^U(\rho)$$

with the abbreviations:

$$\rho = kr = (2\mu E/\hbar^2)^{-1/2} r, \quad \varphi_l{}^U(\rho) = rR_l(r),$$

$$D_\rho{}^U = \rho^2[d^2/d\rho^2 + 1 - U(\rho)], \quad U(\rho) = V(r)/E.$$

The potential $U(\rho)$ is the unknown quantity which has to be calculated from the phases δ_l of the radial wave functions $\varphi_l{}^U(\rho)$ at fixed energy. According to Newton[1-3] the functions $\varphi_l{}^U(\rho)$ fulfill the coupled system of equations:

$$\varphi_l^U(\rho) = \varphi_l{}^{U_0}(\rho) - \sum_{l'=0}^{\infty} c_{l'}{}^U L_{ll'}(\rho)\varphi_{l'}{}^U(\rho), \quad (3)$$

$$L_{ll'}(\rho) = \int_0^\rho \varphi_l{}^{U_0}(\rho')\varphi_{l'}{}^{U_0}(\rho')\frac{d\rho'}{\rho'^2}. \quad (4)$$

The functions $\varphi_l{}^{U_0}(\rho)$ are the regular solutions of the radial Schrödinger equation for a given reference potential U_0:

$$D_\rho^{U_0}\varphi_l^{U_0}(\rho) = l(l+1)\varphi_l^{U_0}(\rho). \tag{5}$$

Equation (3) is used twice, namely, to calculate the coefficients c_l^U from the phases, as discussed below, and, further, to obtain afterwards the functions $\varphi_l^U(\rho)$ at all values of ρ. The resulting coefficients c_l^U and functions $\varphi_l^U(\rho)$, are inserted in the following relation for the potential:

$$U(\rho) = U_0(\rho) - \frac{2}{\rho}\frac{d}{d\rho}\left(\frac{K_{U_0}^U(\rho,\rho)}{\rho}\right), \tag{6}$$

$$K_{U_0}^U(\rho,\rho') = \sum_{l=0}^{\infty} c_l^U \varphi_l^{U_0}(\rho')\varphi_l^U(\rho). \tag{7}$$

The mathematical proof of this result is given in literature.[2,3]

To relate Eq. (3) with the phases one demands the following asymptotic behavior for the wave functions ($\rho\to\infty$):

$$\varphi_l^{U_0}(\rho) = \sin(\rho - \tfrac{1}{2}l\pi + \sigma_l - \eta\ln 2\rho), \tag{8}$$

$$\varphi_l^U(\rho) = A_l^U \sin(\rho - \tfrac{1}{2}l\pi + \delta_l - \eta\ln 2\rho). \tag{9}$$

Here, σ_l and δ_l are the phases of the potentials U_0 and U, respectively. We included also the shift due to a Coulomb potential for the scattering of charged particles $[\eta = \mu Z Z' e^2/(2\mu E\hbar^2)^{1/2}]$. In the Newton-Sabatier method equations for the unknown coefficients A_l^U and c_l^U are obtained by inserting the asymptotic wave functions (8) and (9) into Eq. (3) and equating terms proportional to $\exp(\pm i\rho)$.

Modification of the Newton method.—In most problems of physics, e.g., in atomic and nuclear physics, the potential is known from a finite distance $\rho=\rho_0$ up to infinity, say $U(\rho)=U_0(\rho)$. Therefore, we require that $U(\rho)$ converges to $U_0(\rho)$ for $\rho>\rho_0$:

$$U(\rho) = U_0(\rho) + \Delta U(\rho). \tag{10}$$

The additional term $\Delta U = -2\rho^{-1}d(K/\rho)/d\rho$ should approach zero for $\rho>\rho_0$. It assures that $U(\rho)$ is an analytic function and belongs to the set of solutions (6) of Newton's method. Using physical arguments we neglect ΔU. Then the wave function (9) can be expressed for $\rho>\rho_0$ in terms of the regular and irregular solutions of Eq. (5), denoted as $F_l(\rho)$ and $G_l(\rho)$, respectively. We obtain for $\rho>\rho_0$,

$$\varphi_l^{U_0} = F_l(\rho), \tag{11}$$

$$\varphi_l^U = A_l^U[\cos(\delta_l-\sigma_l)F_l(\rho) + \sin(\delta_l-\sigma_l)G_l(\rho)]. \tag{12}$$

The asymptotic behavior of the functions is given by Eqs. (8) and (9). In the case of $U_0=0$ they are spherical Riccati-Bessel functions: $F_l=\rho j_l(\rho)$, $G_l=-\rho n_l(\rho)$. Inserting (11) and (12) into Eqs. (3) we obtain a set of coupled equations for the coefficients A_l^U and $b_l^U = c_l^U A_l^U$ $(\rho>\rho_0)$:

$$\sum_{l'=0}^{\infty}[\delta_{ll'}T_{l'}(\rho)A_{l'}^U + L_{ll'}(\rho)T_{l'}(\rho)b_{l'}^U] = F_l(\rho), \quad T_l(\rho) = \cos(\delta_l-\sigma_l)F_l(\rho) + \sin(\delta_l-\sigma_l)G_l(\rho). \tag{13}$$

The coefficients A_l^U and b_l^U may depend weakly on ρ, since we have neglected the very small effect of $\Delta U(\rho)$ on φ^U. We limit the number of l values to $l\le L$ and write Eq. (13) as

$$\sum_{l'=0}^{L}(M_{ll'}^{(1)}(\rho)A_{l'}^U + M_{ll'}^{(2)}(\rho)b_{l'}^U) = F_l(\rho), \tag{14}$$

for $l=0, \ldots, L$, where

$$M_{ll'}^{(1)}(\rho) = \delta_{ll'}T_{l'}(\rho), \quad M_{ll'}^{(2)}(\rho) = L_{ll'}(\rho)T_{l'}(\rho). \tag{15}$$

To obtain the $2(L+1)$ coefficients A_l^U, b_l^U the equations may be solved at two radial distances $\rho=\rho_1,\rho_2$ $(>\rho_0)$. Since the resulting coefficients depend on the chosen values of ρ_1 and ρ_2 mainly because of the finite size of the system of Eqs. (14), we suggest a least-squares method[8] for an optimum solution of Eqs. (14).

Least-squares method.—Let us search for an optimum solution of Eqs. (14) at N points $\rho=\rho_1,\rho_2,\ldots,\rho_N$ $(\rho_i>\rho_0)$. The overdetermined system of equations for the unknown vector X is given by

$$M\cdot X = F, \tag{16}$$

where

$$X=\begin{bmatrix} A_0^U \\ \cdot \\ \cdot \\ \cdot \\ A_L^U \\ b_0^U \\ \cdot \\ \cdot \\ \cdot \\ b_L^U \end{bmatrix}, \quad F=\begin{bmatrix} F_1 \\ \cdot \\ \cdot \\ \cdot \\ F_N \end{bmatrix}, \quad F_i=\begin{bmatrix} F_0(\rho_i) \\ \cdot \\ \cdot \\ \cdot \\ F_L(\rho_i) \end{bmatrix}, \quad M=\begin{bmatrix} M^{(1)}(\rho_1) & M^{(2)}(\rho_1) \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ M^{(1)}(\rho_N) & M^{(2)}(\rho_N) \end{bmatrix}.$$

The matrices $M^{(1)}(\rho)$ and $M^{(2)}(\rho)$ are defined in Eqs. (15). M is a matrix with $2(L+1)$ columns and $N\times 2(L+1)$ rows; X is a vector with $2(L+1)$ components and F a vector with $N\times 2(L+1)$ components. The optimum vector X, which minimizes the norm $\|MX-F\|$, is finally obtained as follows[9]:

$$X=(M^\dagger M)^{-1}M^\dagger F, \qquad (17)$$

where $M^\dagger$ is the Hermitian adjoint matrix of M.

Proof of the uniqueness of the solution for $U_0=0$.—First we prove for U_0 that the condition (10) is sufficient for a unique solution of Newton's equations. For $U_0=0$ Redmond[8] has shown that the infinity of equivalent potentials, which yield the same phases at a fixed energy, depends only on one parameter. Sabatier[10] has shown for $U_0=0$ that, if the phase shifts go to zero faster than l^{-3} as $l\to\infty$, there exists one potential and only one, which goes to zero faster than $\rho^{-2+\epsilon}$ as $\rho\to\infty$, whereas all the equivalent potentials are damped by a factor $\rho^{-3/2}$. Therefore, the condition (10) selects a unique potential out of the one-parameter infinity of equivalent potentials.

Next we prove that Eqs. (13) yield $U(\rho)=U_0(\rho)$ for $\rho>\rho_0$. For this we derive the following relation from Eq. (3), with use of Eqs. (4) and (7) and the method given by Newton[1]:

$$K^2(\rho,\rho)=\rho^2\sum_{l=0}^{\infty}c_l^U\left(\varphi_l^U\frac{d\varphi_l^{U_0}}{d\rho}-\varphi_l^{U_0}\frac{d\varphi_l^U}{d\rho}\right). \qquad (18)$$

For $\rho>\rho_0$ we insert the functions (11) and (12) into (18). We obtain a relation which can also be derived from Eqs. (13), if we assume that A_l^U and b_l^U are independent of ρ [i.e., $\Delta U=0$ in Eq. (10)]:

$$K^2(\rho,\rho)=\rho^2\sum_{l=0}^{\infty}b_l^U\sin(\delta_l-\sigma_l). \qquad (19)$$

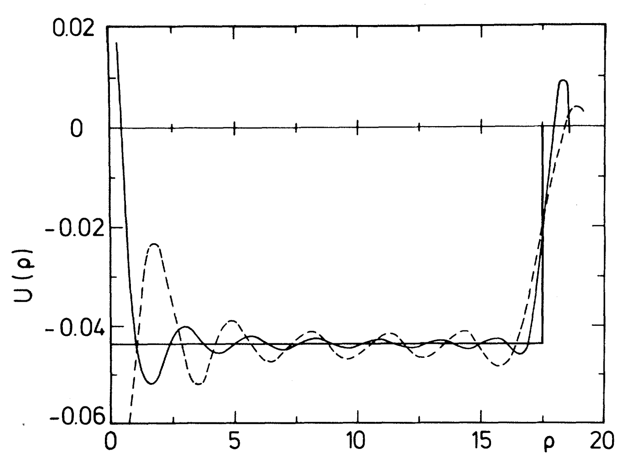

FIG. 1. Comparison of calculations with the modified Newton method (solid line) and by Coudray (dashed line) (Ref. 5) for the square well potential shown in the figure.

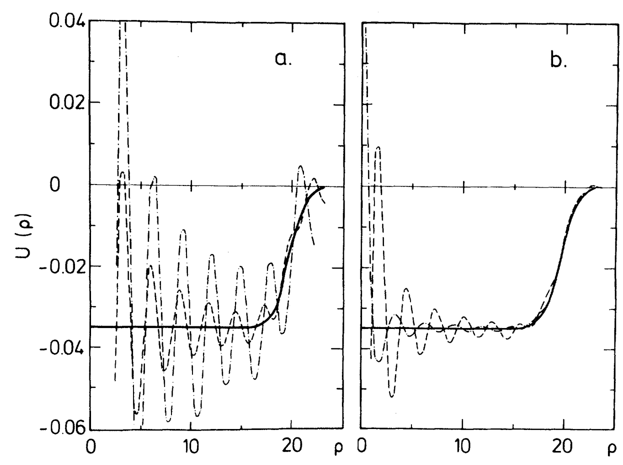

FIG. 2. Calculation of a potential from the first 24 phases of a real Saxon-Woods potential shown in the figure. The parameters are as follows: (a) $N=2$, $\rho_i=24$ and 25 (dashed line); $N=2$, $\rho_i=27$ and 30 (dot-dashed line). (b) $N=3$, $\rho_i=24$, 25, and 26 (dashed line); $N=4$, $\rho_i=24$, 25, 26, and 27 (dot-dashed line).

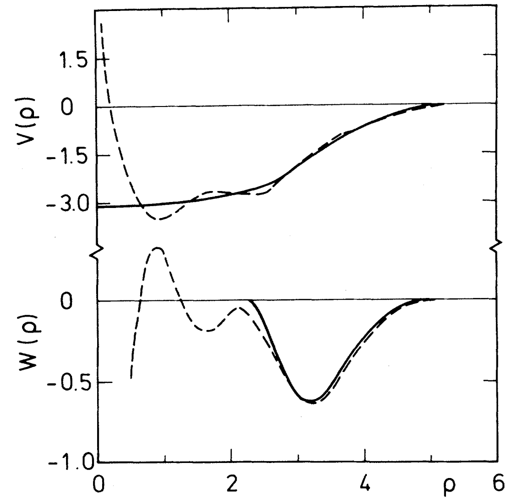

FIG. 3. Calculation of a complex potential $V + iW$ (dashed line) from the first fourteen phases of a potential (solid line) given in Ref. 11 ($E_{c.m.}$ = 14 MeV). The parameters are $N = 3$, ρ_i = 6, 7, and 8.

When Eq. (19) is inserted into Eq. (6), it yields $U(\rho) = U_0(\rho)$ for $\rho > \rho_0$. Hence, the coefficients A_l^U and b_l^U, which fulfill Eqs. (13), belong to a potential $U(\rho) - U_0(0)$ which goes to zero faster than $\rho^{-3/2}$ for $\rho \to \infty$. Therefore, according to the theorems of Redmond and Sabatier stated above, this potential is the unique solution of the problem in the case of $U_0 = 0$.

Results.—We have tested the modified Newton method for the scattering of neutral particles with phases of given potentials. For simplicity we have set $U_0 = 0$. In Fig. 1 we compare our results with that of Coudray[5] (Newton-Sabatier method) for the same square-well potential and energy. It demonstrates the satisfactory applicability of our method. In this calculation we have chosen $\rho_1 = 18$, $\rho_2 = 19$ [$N = 2$, no overdetermined system of Eqs. (16)] and 20 phases ($L = 19$) in comparison to 28 phases taken by Coudray. In Fig. 2(a) we illustrate the dependence of the method on the choice of ρ_1 and ρ_2 for $N = 2$ and in Fig. 2(b) the obvious improvement by the least-squares method for $N = 3$ and 4 for a real potential of Saxon-Woods type. Also we obtained very satisfactory results with complex optical potentials. As a more sensitive test of our method, we computed the potential from the phases of a realistic optical potential with surface absorption which has been used by Wilmore and Hodgson[11] to describe the elastic scattering of neutrons on ^{32}S at $E_{c.m.} = 14$ MeV. With fourteen phases ($L = 13$) and $N = 3$ we obtained the real and imaginary potentials shown in Fig. 3. The potentials agree in the surface region and can be improved in the volume region by taking more phases into account.

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