International Journal of Theoretical Physics, Vol. 41, No. 9, September 2002 (© 2002)

Potential Identification by Inverse Scattering Theory

A. Zerarka[1,2] and Y. Boumedjane[1]

Received January 18, 2002

In the context of JWKB (Jeffreys, Wentzel, Kramers, and Brillouin) approximation, we use inverse scattering theory to modify the forbidden region by introducing an arbitrary term in the analytical expression of the potential $\nu(r)$ in the case of He-Na elastic scattering given as an example.

KEY WORDS: JWKB; phase shift; scattering.

1. INTRODUCTION

Inverse problems are actively studied in the areas of pattern recognition, identification, and optimization theory.

Some inverse problems can also be formulated in the framework of scattering theory. This approach is beginning to play an ever-increasing role in forming numerical algorithms, especially when dealing with complicated problems of physics in which it is difficult to estimate a priori the effects of various factors on the solution of the problem.

The deduction of the interaction from structural data obtained from scattering experiments has been the object of much attention. Important results in this direction have been achieved (Bellisent-Funel *et al.*, 1989; Dharma-Wardana and Aers, 1986; Dzugutov *et al.*, 1988; Kahl *et al.*, 1996; Kahl and Kristufek, 1994; Levesque *et al.*, 1985; Reatto *et al.*, 1986) in the physics of liquid and collisions.

We try to identify the potential with a known structure in terms of information provided by some elements of the data (functionals) regarding the process and to analyze and control the process.

The main objective of this work is to show how the unreachable part of the potential $\nu_2(r)$ in the work of Cao and Zerarka (1985) may be avoided by including an auxiliary term in the potential $\nu(r) = \nu_1(r) + \nu_2(r)$, in which the first

---

[1] Département de physique, Université de Biskra, Biskra, Algeria.

[2] To whom correspondence should be addressed at Départment de physique, Université de Biskra, B P 145, 07000 Biskra, Algeria; e-mail: azerarka@hotmail.com.

0020-7748/02/0900-1745/0 © 2002 Plenum Publishing Corporation

term represents the Van der Waals attractive interaction and the second one is repulsive and describes the exchange effect of the atomic electrons.

The partial phase shift $\delta_a^1(l)$ corresponding to the arbitrary potential is known, but the total partial phase shift $\delta(I)$ for $\nu(r)$ remains unchanged and can also be calculated analytically in terms of $\delta_a^1(l)$, $\nu_1(r)$, and the auxiliary potential. An analytical expression of $\nu_2(r)$ is obtained by a similar way as in Cao and Zerarka. For the sake of clarity, the paper is organized as follows. Section 2 is devoted to a summary of those aspects of semiclassical method that are directly pertinent to the analytical expression of the phase shift. In Section 3, the potential $\nu_2(r)$ is investigated by using the inverse scattering theory. In Section 4, an application for the case of He-Na elastic scattering is presented and numerical results and conclusion are presented in Section 5.

2. PHASE SHIFT

The JWKB (Froman, 1965) phase shift may be obtained by using the radial part of the Schrödinger equation

$$\Delta\psi + K_1^2(r)\psi = 2\mu\nu_2(r)\psi \tag{1}$$

where

$$K_1^2(r) = 2\mu[E_0 - l(l+1)/r^2 - \nu_1(r)] \tag{2}$$

in which E_0 and μ represent, respectively, the incident energy and the reduced mass, and $\hbar$ has been set equal to unity.

We have calculated the potential $\nu_2(r)$ by the JWKB inverse scattering theory and we have shown that the inner region ($r < 7.80$) is nonaccessible; it does correspond to the forbidden one. In order to solve these difficulties, it is always possible to impose an auxiliary potential $\nu_a(r)$, which respects the conditions of validity of JWKB approximation for a fixed energy. The simplest idea is to modify the potential $\nu(r)$ in such a way that it preserves the same form. We can rewrite the potential $\nu(r)$ by introducing an arbitrary $\nu_a(r)$ leading to a new form of $\nu(r)$ as

$$\nu(r) = \nu_a(r) + V_2(r) \tag{3}$$

where

$$V_2(r) = \nu_1(r) + \nu_2(r) - \nu_a(r) \tag{4}$$

A transformation is now possible if we replace $\nu_1(r)$ by $\nu_a(r)$ and $\nu_2(r)$ by $V_2(r)$. The Schrödinger equation then takes the form

$$\Delta\psi + K_{1a}^2(r)\psi = 2\mu V_2(r)\psi \tag{5}$$

$$K_{1a}^2(r) = 2\mu[E_0 - l(l+1)/r^2 - \nu_a(r)] \tag{6}$$

A similar way as in Cao and Zerarka, we write the phase shift $\delta(l)$ by using the specific conditions of validity of the JWKB approach:

$$\delta(l) = \delta_a^1(l) - \mu \int_{r_0}^{\infty} dr' \frac{V_2(r')}{K_{1a}(r')} \tag{7}$$

where r_0 is the classical turning point, defined by $K_{1a}^2(r) = 0$.

3. DETERMINATION OF POTENTIAL $\nu_2(r)$

In this section we derive an analytical form of potential $\nu_2(r)$ by the inversion process in which the use of Abel transformation is necessary (Cameron, and McKee, 1983; Cao, 1978; Miller, 1969). The potential $\nu_2(r)$ will be expressed by an integral which may be numerically calculated in the frame of the elastic scattering. However the potential $\nu_2(r)$ is directly extracted from $V_2(r)$.

We now define the following practical quantities:

$$p_a(E_0, l) = -\sqrt{2/\mu}\left[\delta(l) - \delta_a^1(l)\right] \tag{8}$$

$$D(E_0, Y) = V_2(r)\frac{dr^2}{dY^2} \tag{9}$$

where

$$Y^2 = r^2(E_0 - \nu_a(r)) \tag{10}$$

The relation (6) may be transformed as

$$K_{1a}(r) = \sqrt{2\mu}\frac{1}{r}\left[Y^2(r) - Y^2(r_0)\right]^{1/2} \tag{11}$$

From (8) the relation (7) becomes

$$P_a(E_0, l) = \int_{Y_0}^{\infty} dY \frac{D(E_0, Y)Y}{(Y^2 - Y_0^2)^{1/2}} \tag{12}$$

To extract the function $D(E_0, Y)$, we need thus the Abel transformation. From (12), we have

$$D(E_0, Y) = -\frac{2}{\pi}\int_{Y}^{\infty} dY_0 (Y_0^2 - Y^2)^{-1/2} \frac{dP_a(E_0, l)}{DY_0} \tag{13}$$

then, the potential $\nu_2(r)$ becomes

$$\nu_2(r) = D(E_0, Y)\left[E_0 - \nu_a(r) - \frac{r}{2}\frac{d\nu_a(r)}{dr}\right] - \nu_1(r) + \nu_a(r) \tag{14}$$

4. APPLICATION TO THE CASE OF He-Na ELASTIC SCATTERING

The case of elastic scattering between He and alkaline atoms like Na may be numerically tested by using the above results.

For those scattering types, the potential $\nu_1(r)$ is assumed to be known a priori, and equal to $-c_6 \cdot r^{-6}$ in which c_6 represents the van der Waals constant and has been computed by Mahan (1969), for different molecular states, whereas the potential $\nu_2(r)$ is controvertible and it is then proposed that it would take the form

$$\nu_2(r) = dr^{\beta}e^{-\alpha r}$$

where $d = 0.015$; $\alpha = 0.94$; $\beta = 2.20$. These values can be found in Roueff (1974). In addition, the arbitrary potential $\nu_a(r)$ is chosen as:

$$\nu_a(r) = ar^{-2}$$

a being a positive or negative constant. Note that, we have taken into account this choice, since we have at our disposal an analytical expression of phase shift $\delta_a^1(l)$ corresponding to this potential (Cao and Tran, 1976) given by

$$\delta_a^1(l) = \frac{\pi}{4}\left[(2l+1)^2 - \sqrt{(2l+1)^2 + 8\mu a}\right] \tag{15}$$

The calculations of the integral $D(E_0, Y)$ allows us to suggest immediately two important criteria on the choice of the parameter a in the potential $\nu_a(r)$.

i) The forbidden region must be sufficiently reduced.
ii) The condition of validity of the JWKB approximation must be always verified.

Note that for the one fixed parameter a, we have to compute the integral $D(E_0, Y)$ via eq. (12) for some values of the turning point.

5. RESULTS AND DISCUSSION

The discrete data of $\delta(I)$ allows us to use the interpolation algorithm, specified on some values of orbital quantum I, based on Newton interpolation polynomials.

Table I. Representation of the Classical Turning Points r_0 Defined by $K_{1a} = 0$ and the Integral $D(E_0, Y)$ in Terms of the Orbital Quantum I, for the Case $a = 0.86 \times 10^{-3}$.

I	r_0	$D(E_0, Y)$
20	4.00	−0.807
25	6.18	0.523
30	7.33	0.415
35	8.58	0.192
40	9.78	0.085

The results of the integral $D(E_0, Y)$ and the turning point r_0 are listed in Tables I–III. The integral is implemented numerically with a standard Simpson integration, by using a Fortran library routine. Results on Figs. 1–3 indicate that the numerical solutions of the potential $v_2(r)$ are in good agreement with the analytical solutions Note also that all curves are plotted by exponential interpolation by using the best fit method for determinig trends in data. As we have already mentioned in Section 1 the particular interest is to reduce the forbidden region by JWKB method. This is mainly due to the fact that $K_{1a}(r)$ becomes imaginary. We have reconstructed the potential with the values of the parameter a, suitably chosen. For example, we see in Fig. 1 that both potentials are similar and the small approach distance is $r = 4.91$. However, in Figs. 2 and 3 the curves are similar within a certain range. From a general point of view, this is justified, since we have supposed that from a certain distance the Exp($\pm i S(r)$) terms give a negligible contribution (Cao and Zerarka, 1985). The values $r = 2.76$ and $r = 2.45$ are the small approach distances in the Figs. 2 and 3, respectively.

We have also presented the potential $v_2(r)$ described in Cao and Zerarka (1985) in an attempt to compare the approach distances with those investigated in this work. According to the previous result, the value $r = 7.8$ is the small approach

Table II. Representation of the Classical Turning Points r_0 Defined by $K_{1a} = 0$ and the Integral $D(E_0, Y)$ in Terms of the Orbital Quantum I, for the Case $a = -0.1$.

I	r_0	$D(E_0, Y)$
36	2.76	−126
37	3.45	−24.72
38	4.04	−6.373
40	5.05	1.745
45	7.10	1.707
50	8.84	1.073

Table III. Representation of the Classical Turning Points r_0 Defined by $K_{1a} = 0$ and the Integral $D(E_0, Y)$ in Terms of the Orbital Quantum I, for the Case $a = -0.5 \times 10^{-3}$.

I	r_0	$D(E_0, Y)$
10	2.45	−288.2
15	3.68	−18.64
20	4.00	−1.143
25	6.11	0.542
30	7.31	0.446
35	8.52	0.219
40	9.73	0.098

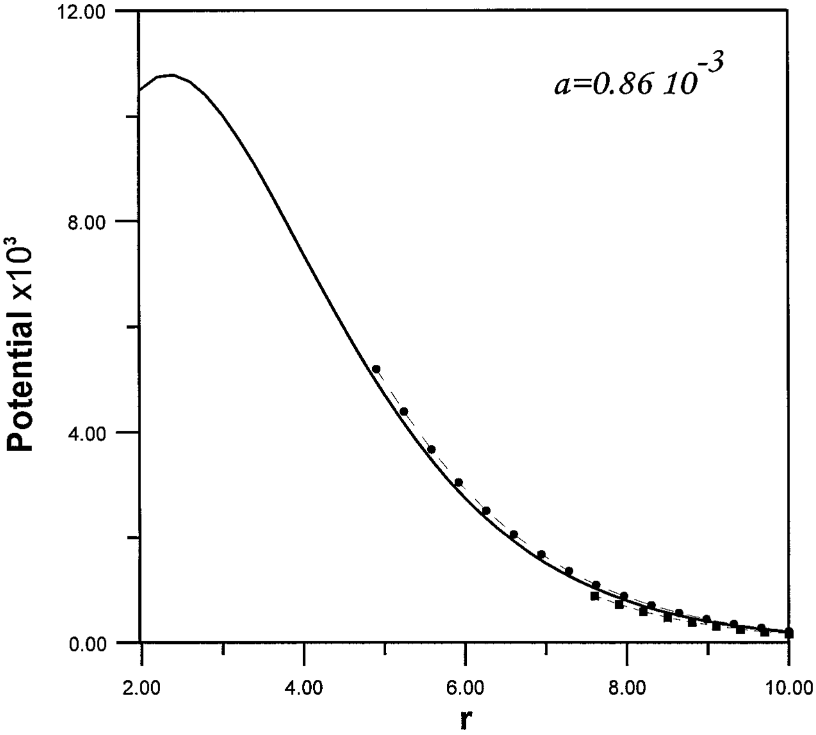

Fig. 1. Representation of potentials $v_2(r)$: full curve, original formula; short broken curve (square), Cao and Zerarka (1985); long broken curve (circle), present result. case: $a = 0.86 \times 10^{-3}$.

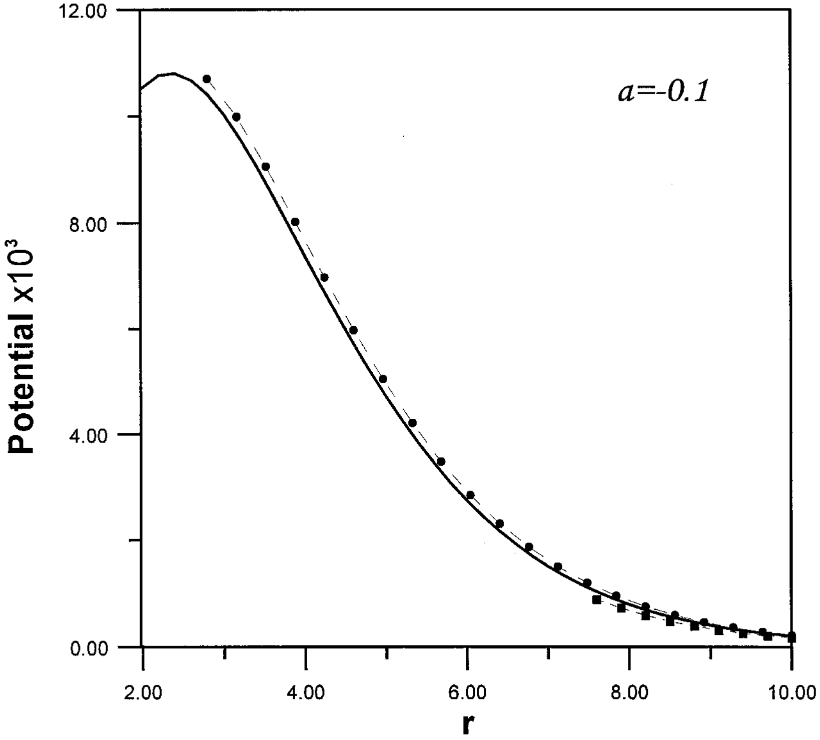

Fig. 2. Representation of potentials $v_2(r)$: full curve, original formula; short broken curve (square), Cao and Zerarka (1985); long broken curve (circle), present result. case: $a = -0.1$.

distance. It now appears clearly that, from these results, the approach distances found by introducing the auxiliary potential $v_a(r)$ may be considered as reference on the choice of the parameter a.

We have therefore shown that for each parameter a the corresponding approach distance permits to reduce the inaccessible part imposed by the JWKB method. We may conclude that it has been possible, using the inverse scattering theory and introducing an arbitrary potential, to reconstruct the potential $v_2(r)$ and to restrict the forbidden interval. We hope that this technique can be employed for a few other parameters or auxiliary potentials. However, the principal difficulty arises from numerical calculations.

ACKNOWLEDGMENTS

The authors acknowledge Pr. R. D. Smith for valuable conversations and useful suggestions.

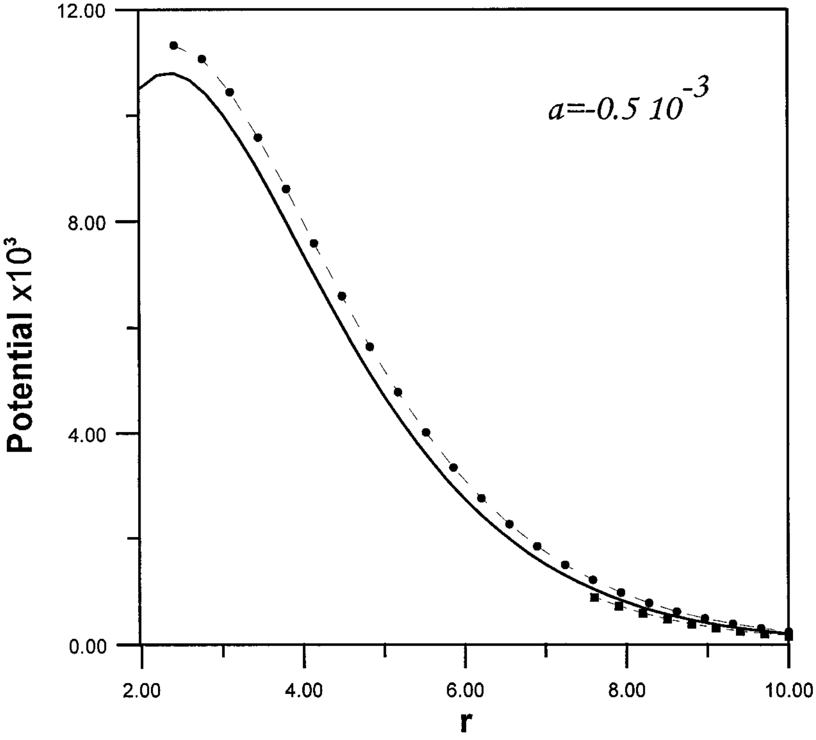

Fig. 3. Representation of potentials $v_2(r)$: full curve, original formula; short broken curve (square), Cao and Zerarka (1985); long broken curve (circle), present result. case: $a = -0.5 \times 10^{-3}$.

REFERENCES

Bellisent-Funel, M. C., Chieux, P., Levesque, D., and Weis, J.-J. (1989). *Physical Review A* **39**, 6310.

Cameron, R. F., and McKee, S. (1983). *International Journal for Numerical Methods in Engineering* 19, 1527–1536.

Cao, X. C. (1985). ICTP Trieste, International Report IC/78/140.

Cao, X. C., and Tran, M. N., (1976). Rapport interne, observatoire de Paris Meudon.

Cao, X. C., Tran, M. N., and Picard, J. (1977). ICTP 2 Paris, p. 607.

Cao, X. C. and Zerarka, A. (1985). ICTP Trieste, International Report IC/85/105.

Dharma-Wardana, M. W. C., and Aers, G. C. (1986). *Physical Review Letters* **56**, 1211.

Dzugutov, M., Larsson, K.-E., and Ebbsjö, I. (1988). *Physical Review A* **38**, 3609.

Froman, P. O. (1965). The JWKB Approximation, North Holland.

Kahl, G. Bildstein, B., and Rosenfeld, Y. (1996). *Physical Review E* **54**, 5391.

Kahl, G., and Kristufek, M. (1994). *Physical Review E* **49**, R3568.

Levesque, D., Weis, J.-J., and Reatto, L. (1985). *Physical Review Letters* **54**, 451.
Mahan, G. D. (1969). *Journal of Chemical Physics* **80**, 2755.
Miller, W. H. (1969). *Journal of Chemical Physics* **51**, 3631.
Reatto, L., Levesque, D., and Weis, J.-J. (1986). *Physical Review A* **33**, 3451.
Roueff, E. (1974). *Journal of Physics B: Atomic, Molecular and Optical Physics* **7**, 185.
Shiff, L. I. (1949). *Quantum Mechanics*, 3rd edn., international student edition.