

**Inverted potential by the phase-integral method: He-Na elastic scattering**

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The phase-integral approximation is used in the frame of the inverse scattering theory to reconstruct a potential of the type  $v = v_1 + v_2$  in which one component  $v_1$  is assumed to be known *a priori*. It is shown that from the knowledge of this term and the phase shift, an analytic expression of the unknown term  $v_2$  can be derived. A number of suggestions in order to enlarge the range of applications of this method are also presented. The case of He-Na elastic scattering is given as an example.

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**I. INTRODUCTION**

Inverse problems are actively studied in the areas of pattern recognition, identification, and optimization theory. Some inverse problems can be also formulated in the framework of the 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 carried out [1–7] in the physics of liquids 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 analyze and control the process.

The main objective of this work is to show in a first part how we rebuild the potential  $v_2(r)$  in the case where the full potential  $v(r)$  is described by  $v_1(r) + v_2(r)$ , in which the first term represents the van der Waals attractive interaction and the second one is repulsive and describes the exchange effect of the atomic electrons. This, is formulated by introducing the phase-integral method. This work shows also how the unreachable part of the potential  $v_2(r)$  may be avoided by including an auxiliary term in the potential  $v(r) = v_1(r) + v_2(r)$ . The partial phase shift corresponding to the arbitrary potential is known, but the total partial phase shift  $\delta(l)$  for  $v(r)$  remains unchanged and can be also calculated analytically in terms of  $v_1(r)$ , and the auxiliary potential.

For the sake of clarity, the paper is organized as follows. Section II is devoted to a summary of the aspects of the semiclassical method that are directly pertinent to the analytical expression of the phase shift. We shall first briefly recall some essential results which will be needed later on in the discussion pertaining to the inverse problem. In Sec. III, an application for the case of He-Na elastic scattering is presented. Section IV will describe the mathematical frame introduced to solve this inverse problem with the use of a phase-integral approach combined with the technique of the Abelian transformation leading to the derivation of a formal relation between  $v_2(r)$ , the first term  $v_1(r)$ , and the phase shift  $\delta(l)$ . The possibility of extension of the present method by introducing an arbitrary potential in the theory is formu-

lated in Sec. V. The numerical results and conclusion are made in Sec. VI.

**II. PHASE SHIFT**

The phase-integral [8,9] phase shift may be obtained by using the radial part of the Schrödinger equation,

$$\Delta \Psi + K_1^2(r) \Psi = 2\mu v_2(r) \Psi, \quad (1)$$

where

$$K_1^2(r) = 2\mu[E_0 - l(l+1)/r^2 - v_1(r)], \quad (2)$$

in which  $E_0$  and  $\mu$  represent, respectively, the incident energy and the reduced mass, and  $\hbar$  has been set equal to unity. The phase-integral solution may be written as

$$\begin{aligned} \Psi(r) = \frac{A}{\sqrt{K_1(r)}} & \left[ c^+(r) \exp\left\{i\left(S_1(r) + \frac{\pi}{4}\right)\right\} - c^-(r) \right. \\ & \left. \times \exp\left\{-i\left(S_1(r) + \frac{\pi}{4}\right)\right\} \right], \end{aligned} \quad (3)$$

where  $A$  is a constant,  $S_1(r) = \int_{r_{01}}^r K_1(r_1) dr_1$ , and  $r_{01}$  is the classical turning point, defined by  $K_1^2(r_{01}) = 0$ . Imposing the condition

$$\begin{aligned} \frac{dc^+(r)}{dr} \exp\left[i\left(S_1(r) + \frac{\pi}{4}\right)\right] \\ - \frac{dc^-(r)}{dr} \exp\left[-i\left(S_1(r) + \frac{\pi}{4}\right)\right] = 0 \end{aligned} \quad (4)$$

to the unknown functions  $c^\pm(r)$  and using the specific conditions of validity of the phase-integral treatment [9], it can be shown that these functions must satisfy a system of coupled first-order differential equations which, in matrix notation, is

$$\frac{dC}{dr} = i\mu \frac{v_2(r)}{K_1(r)} SC, \quad (5)$$

in which the matrices  $C$  and  $S$  are

TABLE I. Values of the quantities  $r_{01}$ ,  $\delta(l)$ , and  $\delta^{(1)}(l)$  in terms of the orbital quantum number  $l$ .

$l$	$r_{01}$ (a.u.)	$\delta^{(1)}(l)$	$\delta(l)$
0			-31.01
5			-23.88
10			-17.93
15			-13.03
20			-9.08
25			-6.00
30			-3.79
35	7.8	+1.40	-2.09
40	9.4	+0.623	-1.06
45	10.7	+0.332	-0.47
50	11.9	+0.193	-0.17
55			+0.019
60			+0.041

$$C = \begin{bmatrix} c^+(r) \\ c^-(r) \end{bmatrix},$$

$$S = \begin{bmatrix} 1 & \exp\left[i\left(S_1(r) + \frac{\pi}{4}\right)\right] \\ \exp\left[-i\left(S_1(r) + \frac{\pi}{4}\right)\right] & -1 \end{bmatrix}.$$

To solve Eq. (5), we may note that generally  $S_1(r)$  is a rapidly increasing function of  $r$  leading to a strong oscillatory character of the exponential term  $\exp[\pm iS_1(r)]$  so that we may use the approximation

$$\int_{r_{01}}^r \frac{v_2(r_1)}{K_1(r_1)} \exp\left[\pm i\left(S_1(r_1) + \frac{\pi}{4}\right)\right] dr_1 \ll \int_{r_{01}}^r \frac{v_2(r_1)}{K_1(r_1)} dr_1, \quad (6)$$

which decouples Eq. (5). Therefore,  $c^\pm(r) = c^\pm(r_{01}) \exp[\mp i\mu \int_{r_{01}}^r v_2(r_1)/K_1(r_1) dr_1]$ , where  $c^\pm(r_{01})$  are the constants to be determined from initial conditions. Furthermore, if  $\delta^{(1)}(l)$  represents the phase-integral phase shift corresponding to the influence of the first term  $v_1(r)$  when the second one is switched off, then from the usual  $S$ -matrix theory, we can extract the following relation:

$$\delta(l) = \delta^{(1)}(l) - \mu \int_{r_{01}}^r \frac{v_2(r_1)}{K_1(r_1)} dr_1. \quad (7)$$

### III. APPLICATION TO THE CASE OF He-Na ELASTIC SCATTERING

The case of elastic scattering between He and alkaline atoms Na may be numerically tested by using the above results. For those scattering types, the potential  $v_1(r)$  is assumed to be known *a priori*, and equal to  $-c_6 r^{-6}$ , in which  $c_6$  represents the van der Waals constant and has been computed by Mahan [10], for different molecular states, whereas the potential  $v_2(r)$  is controvertible and it is then proposed

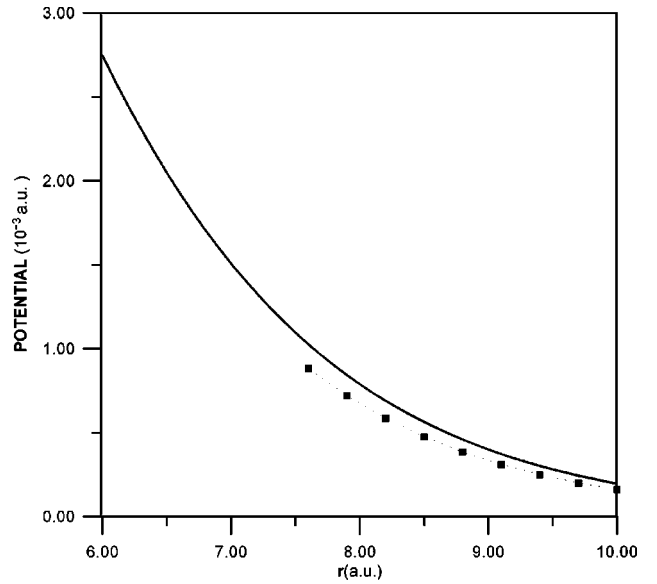


FIG. 1. Representation of potential  $v_2(r)$ , where  $r$  is in a.u. Full curve, original formula; short broken curve (square), standard approach.

that it would take the form  $v_2(r) = dr^\beta e^{-\alpha r}$ , where  $d = 0.015$ ,  $\alpha = 0.94$ , and  $\beta = 2.20$ . These values can be found in Ref. [11] and the present calculations are performed according to these data.

In Table I, we display, in terms of the orbital quantum  $l$ , a number of values of the quantities  $r_{01}$ ,  $\delta(l)$ , and  $\delta^{(1)}(l)$  with the following remarks.

(i)  $r_{01}$  is defined as the largest value of the roots of the equation  $K_1^2(r_{01}) = 2\mu[E_0 - l(l+1)/r_{01}^2 - v_1(r_{01})] = 0$ , and which merely is the turning point corresponding to the potential  $v_1(r)$ .

(ii) The positive and negative signs of the phase shift  $\delta^{(1)}(l)$  merely reflect, as expected, the attractive and repulsive characters of the two components and it can be noticed that the behavior of the phase shift  $\delta(l)$  corresponding to  $v(r)$  is in fact dominated by the influence of the exchange term. Note that, according to our calculations, the phase shift  $\delta(l)$  can be considered as negligible only from  $l > 100$  and that it begins to change sign at  $l = 55$ .

### IV. DETERMINATION OF POTENTIAL $v_2(r)$ : A STANDARD APPROACH

In this section we derive an analytical form of the potential  $v_2(r)$  by the inversion process, in which the use of the Abel transformation [12–14] is necessary. The potential  $v_2(r)$  will be expressed by an integral that may be numerically calculated in the frame of the elastic scattering.

We now define the following practical quantities:

$$P(E_0, l) = -\sqrt{\frac{2}{\mu}} [\delta(l) - \delta^{(1)}(l)], \quad (8)$$

$$D(E_0, Y) = v_2(r) \frac{dr^2}{dY^2}, \quad (9)$$

TABLE II. Representation of the classical turning points  $r_{0a}$  defined by  $K_{1a}(r_{0a})=0$  and the integral  $D_a(E_0, Y)$  in terms of the orbital quantum number  $l$ , for the case  $a=0.86 \times 10^{-3}$ .

$l$	20	25	30	35	40
$r_{0a}$ (a.u.)	4.000	6.180	7.333	8.581	9.780
$D_a(E_0, Y)$	-0.807	0.523	0.415	0.192	0.085

where

$$Y^2(r) = Y^2 = r^2[E_0 - v_1(r)],$$

$$Y^2(r_{01}) = Y_{01}^2 = r_{01}^2[E_0 - v_1(r_{01})]. \quad (10)$$

The relation (2) may be transformed as

$$K_1(r) = \sqrt{2\mu} \frac{1}{r} [Y^2 - Y_{01}^2]^{1/2}. \quad (11)$$

From Eq. (7), relation (8) becomes

$$P(E_0, l) = \int_{Y_{01}}^{\infty} dY \frac{D(E_0, Y) Y}{(Y^2 - Y_{01}^2)^{1/2}}. \quad (12)$$

We may now multiply both members of Eq. (12) by the quantity  $2Y_{01}/\sqrt{Y_{01}^2 - b^2}$  and integrate on  $Y_{01}$  from  $b$  to  $\infty$ , where  $b$  is an arbitrary parameter. We have then

$$\int_b^{\infty} P(E_0, l) \frac{2Y_{01}}{\sqrt{Y_{01}^2 - b^2}} dY_{01} = \pi \int_b^{\infty} D(E_0, Y) Y dY, \quad (13)$$

in which we have used the following relation  $\int_b^Y [2Y_{01}/\sqrt{(Y_{01}^2 - b^2)(Y^2 - Y_{01}^2)}] dY_{01} = \pi$ . Differentiating both members of Eq. (13) in terms of  $b$  and after some partial integration, we obtain

$$D(E_0, Y) = -\frac{2}{\pi} \int_Y^{\infty} \frac{2Y_{01}}{\sqrt{(Y_{01}^2 - Y^2)}} \frac{dP(E_0, l)}{dY_{01}} dY_{01}, \quad (14)$$

and  $b$  has been replaced by  $Y$ .

This result is interesting in the sense that the question of existence and uniqueness of the solution in the inverse problem is implicitly guaranteed here. In fact, it can be shown that the integral in Eq. (14) is always convergent on one hand and, on the other, the unicity of this type of Abel transformation is well known. From Eqs. (9), (10), and (14), the final analytic expression to reconstruct the term  $v_2(r)$  is

 TABLE III. Same as Table II, but  $a = -0.1$ .

$l$	36	37	38	40	45	50
$r_{0a}$ (a.u.)	2.760	3.450	4.041	5.052	7.100	8.841
$D_a(E_0, Y)$	-126	-24.72	-6.373	1.745	1.707	1.073

 TABLE IV. Same as Table II, but  $a = -0.5 \times 10^{-3}$ .

$l$	10	15	20	25	30	35	40
$r_{0a}$ (a.u.)	2.451	3.682	4.001	6.112	7.310	8.520	9.731
$D_a(E_0, Y)$	-288.2	-18.64	-1.143	0.542	0.446	0.219	0.098

$$v_2(r) = D(E_0, Y) \left[ E_0 - v_1(r) - \frac{r}{2} \frac{dv_1(r)}{dr} \right]. \quad (15)$$

In other words, provided that  $v_1(r)$  and  $\delta(l)$  are known, it is always possible to reach  $v_2(r)$  and therefore  $v(r)$ . In order to evaluate  $D(E_0, Y)$  we use the phase shifts given in Table I to obtain  $P(E_0, l)$  in a first step, and then, by interpolation, reach the quantity  $dP(E_0, l)/dl$  in a second step. From the computational point of view, in order to avoid the singularity when  $Y = Y_{01}$ , we use the Buck transformation [15]:  $l^2 - 2\mu Y^2 = z^2$ , which will transform the integral (14) in a more convenient form:

$$D(E_0, Y) = \frac{2}{\pi} \int_0^{\infty} \frac{\exp[-0.36(\sqrt{z^2 + 2\mu Y^2} - 35)]}{\sqrt{z^2 + 2\mu Y^2}} dz; \quad (16)$$

combined with the van der Waals potential for  $v_1(r)$ , we have finally

$$v_2(r) = D(E_0, Y) \left[ E_0 - 2 \frac{c_6}{r^6} \right]. \quad (17)$$

In Fig. 1, we report the results obtained from relation (17) compared to the original curve  $v_2(r) = dr^\beta e^{-\alpha r}$ . Note that the discrepancy between the curves is not surprising but

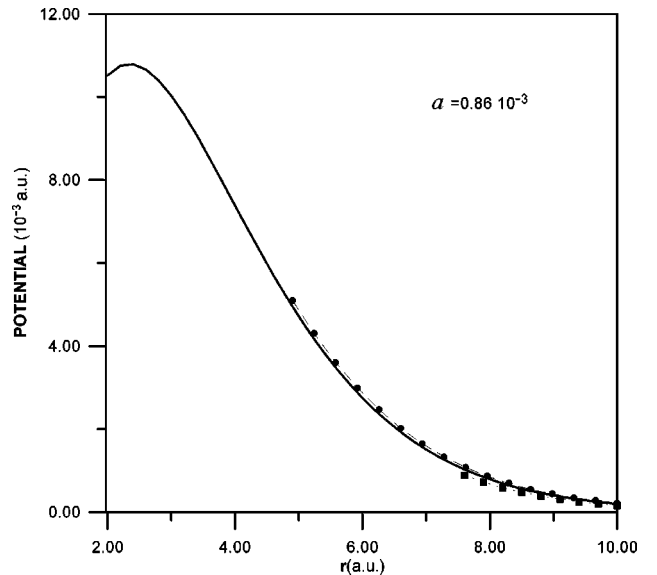
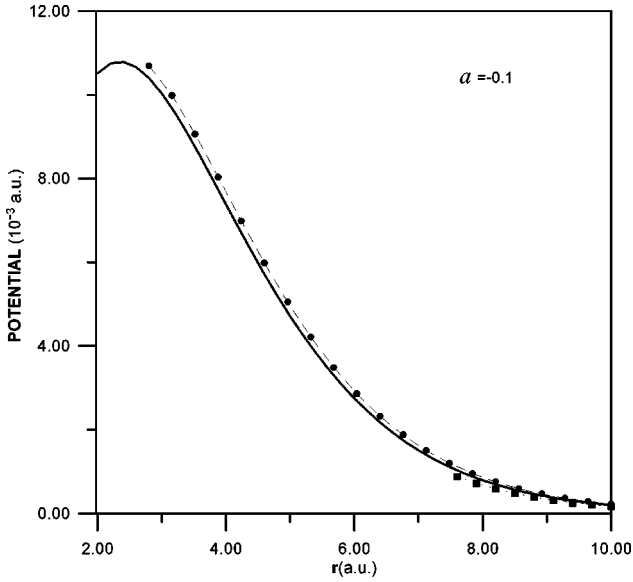


FIG. 2. Representation of potentials  $v_2(r)$ , where  $r$  is in a.u. Full curve, original formula; short broken curve (square), standard approach; long broken curve (circle), result with auxiliary potential for the case  $a = 0.86 \times 10^{-3}$ .


 FIG. 3. Same as Fig. 2, but  $a = -0.1$ .

may be expected from the approximation (6), which has been introduced previously to decouple the differential equations. On the other hand, the inner region where  $r < 7.80$  cannot be reached by the present development because in the frame of a conventional phase-integral approach, it does correspond to the forbidden one. In the following section, the use of a third appropriately chosen auxiliary term in the analytical expression of the potential  $v(r)$  may, in some cases, make accessible a non-negligible part of this region.

### V. THE AUXILIARY POTENTIAL

We have calculated the potential  $v_2(r)$  by the phase-integral inverse scattering theory and have shown that while 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  $v_a(r)$  that respects the conditions of validity of the phase-integral approximation for a fixed energy. The simplest idea is to modify the potential  $v(r)$  in such a way that it preserves the same form.

We can rewrite the potential  $v(r)$  by introducing an arbitrary  $v_a(r)$  leading to a new form of  $v(r)$  as

$$v(r) = v_a(r) + V_2(r), \quad (18)$$

where

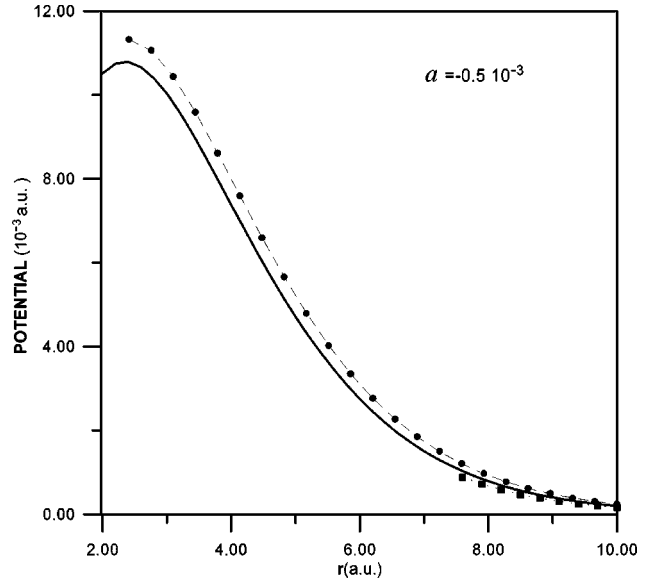
$$V_2(r) = v_1(r) + v_2(r) - v_a(r). \quad (19)$$

A transformation is now possible if we replace  $v_1(r)$  by  $v_a(r)$  and  $v_2(r)$  by  $V_2(r)$ . The Schrödinger equation then takes the form

$$\Delta \Psi + K_{1a}^2(r) \Psi = 2\mu V_2(r) \Psi, \quad (20)$$

where

$$K_{1a}^2(r) = 2\mu[E_0 - l(l+1)/r^2 - v_a(r)]. \quad (21)$$


 FIG. 4. Same as Fig. 2, but  $a = -0.5 \times 10^{-3}$ 

We write  $P_a(E_0, l)$  as function of the phase shifts by using the specific conditions of validity of the phase-integral approach

$$P_a(E_0, l) = -\sqrt{\frac{2}{\mu}} [\delta(l) - \delta^{(a)}(l)], \quad (22)$$

$$D_a(E_0, Y) = -\frac{2}{\pi} \int_Y^\infty \frac{2Y_{01}}{\sqrt{(Y_{01}^2 - Y^2)}} \frac{dP_a(E_0, l)}{dY_{01}} dY_{01}. \quad (23)$$

Now the potential  $V_2(r)$  is extracted from  $D_a(E_0, Y) = V_2(r) dr^2 / dY^2$ , and  $v_2(r)$  is deduced from Eq. (19); then we obtain

$$v_2(r) = D_a(E_0, Y) \left[ E_0 - v_a(r) - \frac{r}{2} \frac{dv_a(r)}{dr} \right] - v_1(r) + v_a(r). \quad (24)$$

### Application to He-Na

The arbitrary potential  $v_a(r)$  is chosen as  $v_a(r) = ar^{-2}$ , where  $a$  is a positive or negative constant. Note that we have taken this choice into account, since we have at our disposal an analytical expression of the phase shift  $\delta^{(a)}(l)$  corresponding to this potential [16] given by

$$\delta^{(a)}(l) = \frac{\pi}{4} [(2l+1)^2 - \{(2l+1)^2 + 8\mu a\}^{1/2}]. \quad (25)$$

The calculations of the integral  $D_a(E_0, Y)$  allow us to suggest immediately two important criteria on the choice of the parameter  $a$  in the potential  $v_a(r)$ : (i) The forbidden region must be sufficiently reduced; (ii) the condition of validity of the phase-integral approximation must always be verified.

## VI. DISCUSSION

The discrete data of  $\delta(l)$  allow us to use the interpolation algorithm, specified on some values of orbital quantum  $l$ , based on Newton interpolation polynomials. The results of the integral  $D_a(E_0, Y)$  and the turning points  $r_{0a}$  are listed in Tables II–IV. The integral is implemented numerically with a standard Simpson integration, by using a FORTRAN library routine. The results in Figs. 2–4 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 determining trends in data.

As we have already mentioned, our particular interest is to reduce the forbidden region by using the phase-integral 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. 2 that both potentials are similar and the small approach distance is  $r=4.91$ . However in Figs. 3 and 4 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 terms give a negligible contribution. The values  $r=2.76$  and  $r=2.45$  are the small approach distances in Figs. 3 and 4, respectively.

We have also presented the potential  $v_2(r)$  described in

the standard approach in the goal to compare the approach distances with those investigated in the case where the auxiliary potential is introduced. According to the previous result, the value  $r=7.8$  is the small approach distance. From these results, it appears now clearly that the approach distances found by introducing the auxiliary potential  $v_a(r)$  may be considered as a reference on the choice of the parameter  $a$ .

We have therefore shown that for each parameter  $a$ , the corresponding approach distance obtained reduces the inaccessible part imposed by the phase-integral method. We may conclude that it has been possible by using the inverse scattering theory and introducing an arbitrary potential to reconstruct the potential  $v_2(r)$  and to restrict the forbidden interval. In a later paper, we apply our approach to very accurate scattering experiments on Kr [17], and the extracted potential is compared with the Lennard-Jones potential with the usual parametrization for Kr [18], the Aziz-Slaman potential [19], and for the Rosen-Morse potentials [20].

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- [1] M. Dzugutov, K-E. Larsson, and I. Ebbsjö, *Phys. Rev. A* **38**, 3609 (1988).
  - [2] D. Levesque, J-J. Weis, and L. Reatto, *Phys. Rev. Lett.* **54**, 451 (1985).
  - [3] M. W. C. Dharma-Wardana and G. C. Aers, *Phys. Rev. Lett.* **56**, 1211 (1986).
  - [4] L. Reatto, D. Levesque, and J-J. Weis, *Phys. Rev. A* **33**, 3451 (1986).
  - [5] M. C. Bellisent-Funel, P. Chieux, D. Levesque, and J-J. Weis, *Phys. Rev. A* **39**, 6310 (1989).
  - [6] G. Kahl and M. Kristufek, *Phys. Rev. E* **49**, R3568 (1994).
  - [7] G. Kahl, B. Bildstein, and Y. Rosenfeld, *Phys. Rev. E* **54**, 5391 (1996).
  - [8] L. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill, New York, 1949).
  - [9] P. O. Froman, *The JWKB Approximation* (North-Holland, Amsterdam, 1965).
  - [10] G. D. Mahan, *J. Chem. Phys.* **80**, 2755 (1969).
  - [11] E. Roueff, *J. Phys. B* **7**, 185 (1974).
  - [12] R. F. Cameron and S. McKee, *Int. J. Numer. Methods Eng.* **19**, 1527 (1983).
  - [13] X. C. Cao, ICTP Trieste International Report No. IC/78/140 (unpublished).
  - [14] W. H. Miller, *J. Chem. Phys.* **51**, 3631 (1969).
  - [15] U. Buck, *J. Chem. Phys.* **54**, 1923 (1977).
  - [16] X. C. Cao and M. N. Tran, Observatoire de Paris Meudon Internal Report No. 22, 1976 (unpublished). X. C. Cao, M. N. Tran, and J. Picard (unpublished).
  - [17] F. Bocchi, P. Chieux, R. Magli, L. Reatto, and M. Tau, *Phys. Rev. Lett.* **70**, 947 (1993); *J. Phys.: Condens. Matter* **5**, 4299 (1993).
  - [18] J.-P. Hansen and I. R. McDonald, *Theory of Simple Liquids*, 2nd ed. (Academic, New York, 1986).
  - [19] R. A. Aziz and M. J. Slaman, *Mol. Phys.* **58**, 679 (1986).
  - [20] N. Dalarsson, *Fiz. B* **3**, 147 (1994).