ENERGY DEPENDENCE OF THE HEAVY IONS POTENTIAL :
α-α AS AN ILLUSTRATIVE CASE

J. CUGNON†

Institut de Physique Nucléaire, Division de Physique Théorique, F-91406 Orsay (France)

Abstract. A local energy-dependent optical potential is constructed for the α-α elastic scattering, taking account of the Pauli principle and of the relative motion. The energy dependence is due partly to the Pauli principle and partly to the nucleon-nucleon force.

† On leave of absence from University of Liège,
Institute of Theoretical Physics,
B-4000 Liège I (Belgium)
1. Introduction

The concept of an optical model potential has proved to be useful in the analysis of elastic heavy ion scattering \(^1\). However, the theoretical calculations of this potential are not yet satisfactory. There are two main approaches to the problem. The first one is based on the definition of the optical model potential as the variation of the potential energy of the system of two ions with their relative distance. This variation may be evaluated using an energy-density formula \(^2\) or using a two centre shell-model \(^3,4\). We refer to these approaches as "static", because they do not account for the relative motion microscopically. In the second class, we put the generator coordinate method and the resonating group method. In these theories, the problem arises to define the optical model potential properly. In the resonating group method, one has the advantage of dealing with an equation for the relative wave function. Unfortunately, in practice, the optical potential can only be defined trivially \(^5\). That introduces non-physical poles in the dependence versus the relative distance. In the generator coordinate methods, the definition of an optical potential is ambiguous \(^6\).

In the last two methods, the optical model potential may be considered as an intermediate (and non necessary) step between the dynamics (i.e. the many-body Hamiltonian) and the cross sections. Nevertheless, the success of the optical model potential for the heavy ion scattering supports the role of the potential scattering in the process. Moreover, the description of the ion-ion interaction by a potential is the most appropriate one to study the molecular-like structure of some states of the system.

In the present paper, we want to investigate the influence of the relative motion on the ion-ion potential. The definition of the potential we adopt here is a generalization of the pres-
scription of the cluster model or of the two centre shell-model. We allow the ions to have a non-zero relative momentum. This method is equivalent to the one proposed by Fliessbach 6). We apply it to the case of alpha-alpha elastic scattering, since this case has been investigated by many methods.

In sect. 2, we briefly recall the definition of the optical model potential. In sect. 3, we give explicit formulae for a nucleon-nucleon force which has the form of the sum of the two gaussians, and we discuss qualitatively the effect of the relative motion. Finally, in sect. 4, we discuss the numerical results. Sect. 5 contains the conclusion.

2. Definition of the optical model potential

We start with the generator coordinate wave functions:

$$|K,D\rangle = N(K,D)\mathcal{A}[(\exp(iK.R_{12})\phi^0_{SM}(-\frac{D}{2})\phi^0_{SM}(-\frac{D}{2})]$$, \hspace{1cm} (2.1)

where \(\phi^0_{SM}(x)\) is the shell-model wave function of a fragment centered at the point \(x\) and where \(R_{12}\) is the relative centre-of-mass coordinate. The operator \(\mathcal{A}\) antisymmetrizes between each cluster. The quantity \(N(K,D)\) is a normalization factor.

The definition of the optical potential proceeds as follows. Let \(K(D)\) be a trajectory in the \(K,D\) space. The optical potential is defined as the variation of the potential energy along this trajectory from infinity to a certain point \(D\):

$$U_{opt}(D) = [h(K(D),D) - \frac{\hbar^2K^2(D)}{2M}]$$

$$- [h(K(\infty),\infty) - \frac{\hbar^2K^2(\infty)}{2M}]$$, \hspace{1cm} (2.2)

where

$$h(K,D) = \langle K,D|H|K,D\rangle$$, \hspace{1cm} (2.3)

while \(M\) is the reduced mass of the system. The trajectory is determined by assuming that (2.2) is a good definition, i.e. that the following energy conservation low holds along the trajectory:
\[
\frac{K^2 \kappa^2(D)}{2M} + U_{\text{opt}}(D) = E_{K,0}.
\]

The quantity \( E_{K,0} \) is the asymptotic kinetic energy. The trajectory \( K(D) \) can be regarded as the mean trajectory along which the wave packet propagates. Eqs. (2.2) and (2.4) define the potential in a self-consistent way: one first chooses a function \( K(D) \); one then calculates \( U_{\text{opt}}(D) \) from eq. (2.2); introducing then this value in eq. (2.4), one obtains another function \( K(D) \), that one puts back in eq. (2.2), etc. until convergence is reached. Below, we neglect the dependence upon the angle between \( K \) and \( D \), assuming no angular momentum dependence, as it is usually done in the two centre shell-model and we can thus use scalar quantities. For \( D \rightarrow \infty \), eqs. (2.2) and (2.4) show that the optical potential approaches zero and that \( K(D) \) tends to the physical asymptotic relative momentum. The connection between the optical potential (2.2) and the generator coordinate formalism has been investigated in ref. 6.

3. Explicit formulae

Here, we evaluate the expectation value of the Hamiltonian for the wave function (2.1). We closely follow ref. 7 and rewrite (2.1) as

\[
|K,D> = N(K,D) \mathcal{A}(\phi_I(0)\phi_{II}(D)) ,
\]

with

\[
\phi_I = \prod_{j=1}^{A_I} g_j(r_j), \quad g_j(r) = \exp(iKr/A_I)\phi_I^I(r)
\]

\[
\phi_{II} = \prod_{j=1}^{A_{II}} f_j(r_j), \quad f_j(r) = \exp(-iKr/A_{II})\phi_{II}^{II}(r)
\]

Here, the \( \phi_I^{I,II} \)'s are the single-particle shell-model wave functions. By a Schmidt procedure we can transform the \( g_j \)'s
in functions \( \tilde{g}_j \) which are orthogonal to the \( f_j \)'s. This is very suitable since in second quantized form, we have

\[
|K,D> = N(K,D) \prod_j g^+_j \prod_i f^+_i |0> = \prod_j \tilde{g}^+_j \prod_i \tilde{f}^+_i |0> .
\] (3.2)

One can consider the states \( f_i \) as a filled Fermi sea which remains unchanged during the whole scattering process. Using the usual form of the Hamiltonian

\[
H = \sum_{\ell} \frac{1}{2} t_{\ell}^2 + \sum_{\ell \neq m} \frac{1}{2} v_{\ell m}
\] ,

we can write, with the help of eqs. (2.2) and (2.3),

\[
U_{\text{opt}}(D) = E(K(D),D) - E(K(\infty),\infty) = \Delta E(K(D),D) ,
\] (3.4)

where

\[
E(K,D) = T(K,D) + V(K,D) + V_{\text{tp}}(K,D) ,
\] (3.5)

with

\[
T(K,D) = \sum_j \tilde{g}_j |t| \tilde{g}_j - \frac{\hbar^2 K^2}{2 m_p}
\] ,

\[
V(K,D) = \frac{1}{2} \sum_{j \neq j'} <\tilde{g}_j \tilde{g}_j |v| \tilde{g}_j \tilde{g}_j>_{\text{AS}} ,
\] (3.6a)

\[
V_{\text{tp}}(K,D) = \frac{1}{2} \sum_{i=1}^{A} \sum_{j=1}^{A} \tilde{g}_j f_i |v| \tilde{g}_j f_i>_{\text{AS}} .
\] (3.6b)

The quantity \( m_p \) is the mass of the ion. The quantity \( \Delta T = T(K,D) - T(K,\infty) \) describes the variation of internal kinetic energy of one ion because of the Pauli correlations induced by the presence of the other ion. The quantity \( \Delta V = V(K,D) - V(K,\infty) \) measures the variation of potential energy due to the same correlations. All the Pauli correlations are contained in the function \( \tilde{g}_j \). One can suppress these correlations by
replacing in eqs. (3.6) the $g_j$'s by the $g_\perp$'s. Then, the quantities $\Delta T$ and $\Delta V$ vanish automatically, since the quantities $T(K,D)$ and $V(K,D)$ do not depend upon $D$ any more. Finally, $V_{tp}$ describes the interaction between the two ions. We emphasize that this term is influenced by the Pauli correlations but that it vanishes with infinite separation distance.

For the $\alpha-\alpha$ system, if the functions $\phi_I$, $\phi_{II}$ (eqs. (3.2)) are 0s harmonic oscillator wave functions, the integrals appearing in eqs. (3.6) can be evaluated analytically, using a nucleon-nucleon force of the form:

$$v_{ij} = \sum_{n=1}^{2} v_n \exp(-\frac{r_{ij}^2}{\mu_n^2}) (1 - m_n + m_n P_m),$$

where $P_m$ exchanges the spatial coordinates. Special care must, however, be taken when $U_{opt}(D)$ is larger than $E_{K,0}$. Then, $K^2$ is negative, by eq. (2.4). One can replace $K$ by $iK$ in eqs. (3.1b) and (3.1c), but the Schmidt procedure is then more complicated because the functions $f_j$ (see eq. (3.1)) are no longer orthogonal (except for the $\alpha-\alpha$ case). Additional terms should appear in eqs. (3.6a) and (3.6b).

Of course, the results are equal for $K^2$ or $\kappa^2 + 0$. As a matter of fact, if we use (3.4) for $K(D) = K(\infty) = 0$, we obtain the adiabatic value of the potential, which contains the effect of the Pauli principle for each value of $D$. By this we mean the following. Let us for instance take two $\alpha$-particles from infinity and bring them at a certain relative distance $D$ and fix them at this position. The Pauli principle forces the occupation of the shells to change. For instance, if $D = 0$, four particles are promoted from the 0s to the 0p-shell. This process takes a finite time. In a real collision, which can be considered as described by the states (2.1) (when the relative distance is equal to $D$), the shells are not rearranged like in the case when the ions are at rest. This is reflected by the fact that the overlap between the $g_j$ and
the \( f_i \) is different from the overlap between the \( \phi_j^{II} \) and the \( \phi_i^{I} \). In fact, as \( K \) tends to infinity, the \( g_j \) and \( f_i \) no longer overlap whatever the value of \( D \) is: this expresses that the Pauli principle is relaxed by the relative motion. In the adiabatic approximation, the relaxation of the Pauli principle is inexistant. We have

\[
U_{ad}(D) = E(0,D) - E(0,\infty)
\]  

(3.8)

On the other hand, we can find the sudden value of the potential by setting \( K(D) = K(\infty) = \infty \) in eq. (3.4). This corresponds to an infinitely rapid collision. We have

\[
U_{sud}(D) = E(\infty,D) - E(\infty,\infty) \\
= \sum_{n=1}^{2} V_n \left( \frac{\mu_n}{b} \right)^3 \left[ \left( \frac{\mu_n}{b} \right)^2 + 2 \right]^{-\frac{3}{2}} (16 - 20 \frac{m_n}{b}) \\
\exp \left( -\frac{D^2}{b^2} \frac{1}{\left( \frac{\mu_n}{b} \right)^2 + 2} \right) 
\]  

(3.9)

In this case, the Pauli principle is completely relaxed and only the \( V_{tp} \) term in eq. (3.5) has a non-vanishing contribution in the sudden case. We come back to this point later.

We stress that our sudden and adiabatic potentials should not be confused with the sudden and adiabatic potentials as defined in the two centre shell-model (see ref. 3 for instance). As the two ions are coming near each other, the shells are distorted by the nuclear interaction: the dynamical correlations and the occupation of the shells are changed because of the Pauli correlations. The relative motion modifies the effect of both types of correlations. In the two centre shell-model, the two ions are always considered at rest, and, thus, the potential is always an adiabatic approximation inasmuch as the Pauli correlations are concerned. In our approach, the potential is al-

ways sudden with respect to the dynamic correlations since we neglect the deformation of the fragments. In Fig. 1, we illustrate our discussion. Our potentials (3.8) and (3.9) are indicated by crosses and the potentials extracted from the two centre shell-model are denoted by circles. This figure also shows that our adiabatic potential is equivalent to the sudden potential of the two centre shell-model. The empty square in Fig. 1 should correspond to a very rapid collision between very soft ions.

4. Numerical results

Here, we present the results of a calculation for the case α-α. The optical potential has been computed for two different forces, the Brink and Boeker B1 force \(^8\) and the Volkov V2 force \(^9\), with, for the latter, the parameters: \(V_1 = + 60\) MeV, \(V_2 = -60\) MeV, \(\mu_1 = 1.01\) fm, \(\mu_2 = 1.80\) fm, \(m_1 = m_2 = 0.6\). The oscillator parameter \(b\) is equal to 1.36 fm.

4.1. Optical_model_potential

Fig. 2 shows the results of the calculation using the B1 force. The potential is attractive at long distances and repulsive at short distances. This repulsion is an essential feature of the Pauli principle. By switching off the Pauli correlations (i.e. putting \(\bar{g}_j\) instead of \(g_j\) in eqs. (3.6)), one obtains a fully attractive potential with a maximum depth of 60 MeV for \(E_{K,0} = 1\) MeV. One can see that the potential is not very energy-dependent in the range \(E_{\text{Lab}} = 0\) to 40 MeV. This can be checked as follows. For a fixed value of \(D\), eqs. (2.4) and (3.4) show that \(U_{\text{opt}}(D)\) is the intersection point of the curve \(U_{\text{opt}} = \Delta E(K,D) = f(K^2)\) with the straight line \(U_{\text{opt}} = \frac{K^2}{2M} + E_{K,0}\) in the \((U_{\text{opt}},K^2)\) plane. The inspection of the curves (not displayed in the figures) \(f(K^2) = \Delta E(K,D = 0)\), and \(f(K^2) = \Delta E(K,D = 3\) fm) (around the minimum) shows that
i) the optical potential remains approximately constant at
D = 0 and D = 3 fm between 0 and 40 MeV. ii) At higher
energies, the potential decreases slowly to reach a shallow
minimum and then goes up. iii) When $K^2$ passes through 0
(K passes from real to pure imaginary), the quantity $\Delta E(K, D)$
is continuous, but not its derivative (hence, the small angular
points in the curves of Fig. 1 and Fig. 4). This is due to
the fact that, as $K^2$ passes through 0, the norm of the
states $f_j$ and $g_j$ is continuous but not continuously derivable.

We finally emphasize that the potential at zero incident
energy is not equal to the adiabatic energy, since the function
$K(D)$ can be locally different from zero.

Fig. 3 displays the results with the V2 force. The potential is less repulsive at short distances, which is presumably due to the smaller repulsive part of V2; it depends much more upon the energy. If we use the rough approximation
$U_{opt}(D) = U^{(0)}(D) - \alpha(D)E_{CM}$ between 0 and 20 MeV (CM), we
get at D = 0, $\alpha = 0.15$ for the B1 and $\alpha = 2$ for the
V2. Around D = 3 fm, $\alpha = 0.15$ for the B1 and $\alpha = 0.8$
for the V2. We discuss below the interpretation of the
energy dependence.

4.2. Contributions to the optical potential

In Fig. 4, we display the different contributions to the
optical potential. We see that the interaction between the ions
(V_{tp}) is essentially attractive, while the variation of internal
kinetic and potential energy is repulsive. As the two ions
are coming near each other, the V_{tp} term starts increasing
(in modulus) more rapidly than the $\Delta T$ and $\Delta V$ terms. This
can be interpreted as follows: the Pauli principle, mainly in
$\Delta T$ and $\Delta V$, comes into play when the orbitals are overlapping.
However, the nuclear interaction is already effective before
this stage, because of the non-zero range of the nuclear forces. This seems to be a quite general effect independent of the size of the fragments.

If we switch off the $V_{tp}$ term, i.e. the ion-ion interaction, we see from Fig. 4 that the Pauli correlations alone are generating phase shifts. The effect is so large that we believe this result not to be bound to our approximations, although this question is not solved yet 10. The orthogonality scattering model yields a quite similar result. This model assumes that the scattering particle does not experience a potential, but that its wave function must be orthogonal to some wave functions (in general localized and of finite norm). It has been shown that this model generates phase shifts (see ref. 11 and other refs. therein).

4.3. Energy dependence

It is now well accepted that the Pauli correlations are essentially repulsive and that this effect is becoming less and less important as the energy increases. However, we also find that the nucleon-nucleon potential plays a role in the energy dependence. At different energies, the system is particularly sensitive to different Fourier components of the nucleon-nucleon force. For the $B_1$, as the energy increases, the Fourier components are more and more repulsive, while the opposite is true for the $V_2$ force. This is illustrated by Fig. 5 which shows, for each force, the adiabatic potential, neglecting the Pauli correlations and the sudden potential. We have thus thrown away the Pauli correlations, since the sudden potential is not influenced by the latter, and we are left with the nucleon-nucleon force effects only. It is clear that $B_1$ is more and more repulsive while the $V_2$ force is more and more attractive. In the region $0-40$ MeV (Lab), the effect of the force on the energy dependence is of the same order as the effect of the
Pauli correlations. For the Bl force, the two effects practically cancel each other, while for V2, they add coherently. One observes (see refs. 12, 13, 14 and below) that the V2 is closer to the physical situation. In summary, we find that the variation of the optical potential is partly due to the Pauli correlations and partly due to the "excited" Fourier components of the nucleon-nucleon force.

4.4. Phase shifts

In order to test the calculation, our potential has been introduced in a Schrödinger equation in order to calculate the phase shifts. The Coulomb interaction has been included by adding the following term to the nuclear interaction

\[ V_c(D) = \frac{Z_1 Z_2}{2D} (3 - \frac{D^2}{X_a^2}) \quad , \quad 0 < D < X_a \]
\[ = \frac{Z_1 Z_2}{D} \quad , \quad D > X_a \]

where \( X_a \) is the sum of the radii of the two \( \alpha \)-particles. The results for \( L = 0 \) are shown in Fig. 5. The results are quite encouraging. The V2 force gives better results than the Bl force. This agrees with the results of Lumbroso 12).

5. Conclusions

We have computed, in the \( \alpha-\alpha \) case, an optical potential which takes full account of the Pauli principle and of the relative motion. The results are force-dependent. The V2 force is closer to the physical situation and leads to the following conclusions. i) The optical potential is more and more attractive as the energy increases.

ii) The energy dependence is due to the relaxation of the Pauli principle at increasing relative momentum on one hand, and to the selection by the relative motion of certain
Fourier components of the nucleon-nucleon force on the other hand. These two effects are of the same order and are both attractive.

iii) The ion-ion potential is essentially attractive at large distances and repulsive (because of the Pauli principle) at short distances. This is presumably related to the non-zero range of the nucleon-nucleon force.

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References

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Figure captions

Fig. 1. See the text for the explanation.

Fig. 2. Optical model potentials calculated with the B1 force at $E_{\text{Lab}} = 1$ MeV (long dashes), 25 MeV (small dashes), 40 MeV (dash-and-dots). The full curve corresponds to the adiabatic approximation (eq. (3.8)).

Fig. 3. Optical model potentials calculated with the V2 force at $E_{\text{Lab}} = 0$ MeV (small dashes), 7.5 MeV (long dashes). The adiabatic approximation (eq. (3.8)) is represented by the full curve.

Fig. 4. Representation of the different terms of eqs. (3.4) and (3.5) for the optical model potential calculated with the B1 force at $E_{\text{Lab}} = 15$ MeV: $\Delta T$ (small dashes), $\Delta V$ (dash-and-dots), $V_{tp}$ (long dashes). The full potential is represented by the full curve.

Fig. 5. Adiabatic optical model potentials without Pauli correlations (long dashes) and sudden potentials (full curves) for the B1 and V2 forces.

Fig. 6. Comparison between the $l = 0$ experimental phase shifts and those calculated from the theoretical optical model potentials. The full line corresponds to the V2 force and the dots to the B1 force.
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Fig. 3

Fig. 4