

Upper Limits on Polarization Effects in Nuclear Collisions

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Abstract

The increase in cross section for inelastic collisions due to polarization of the target by the projectile has an upper limit in a simple model. The usual treatment of core polarization in nuclear collisions gives a polarization potential which is too large because of the use of perturbation theory and the neglect of dynamic effects, and which is in phase with the direct coupling potential contrary to recent experimental evidence and to channel coupling theory.

1. Introduction

The usual treatment of the collision of nucleons with nuclei involves the application of the distorted wave Born approximation and the adoption of a nucleon–nucleon interaction of definite strength. It turns out in many cases that, if the elastic scattering is used to determine the strength of the nucleon–nucleon interaction, the inelastic scattering is then too small in magnitude by at least a factor of two. This failing led to the core polarization model of Love and Satchler (1967) in which account is taken of the interaction of the incident nucleon with the nucleons in the core of the nucleus as well as with the valence nucleons.

The effect of polarization of the target system by projectiles has long been taken into account in many calculations of the elastic scattering of slow electrons by atoms. The effect on the inelastic scattering has been considered recently and found to be too large in the usual approach through perturbation theory (Mohr 1975). It is shown here that the perturbation theory treatment of core polarization may also seriously overestimate the effect, the more so since the static approximation is implied and correcting for the dynamic effect reduces the scattering still further. Finally it is shown that the effect of channel coupling should also be considered.

2. Improved Treatment of Target Polarization

The state of a system polarized by the field of a projectile is that of the unpolarized system mixed with other states. Physically this implies virtual transitions from the unperturbed state to other states during the collision.

Consider a target system with a valence particle, of coordinates x_v , which has energy eigenstates E_i and eigenfunctions $\psi_i(x_v)$. When this particle is perturbed by the field of a projectile, with coordinates x_p , the mutual potential energy of the two particles being $V(x_{vp})$ where $x_{vp} = |x_v - x_p|$, the perturbed target system has eigenfunctions

$\Psi_i(x_v, x_p)$ related to the unperturbed set by the unitary transformation

$$\Psi_i(x_v, x_p) = \sum_k a_{ik}(x_p) \psi_k(x_v). \quad (1)$$

The a_{ik} are functions of x_p only in the usual static approximation and are generally calculated by perturbation theory. They can be obtained more accurately by diagonalizing the energy matrix with diagonal elements E_i and off-diagonal elements given by

$$v_{ki}(x_p) = \int \psi_k^*(x_v) V(x_{vp}) \psi_i(x_v) dx_v, \quad (2)$$

these being the transition potentials effective in the scattering when target polarization is neglected. When target polarization is taken into account the transition potentials are given by

$$V_{ij}(x_p) = \int \Psi_i^*(x_v, x_p) V(x_{vp}) \Psi_j(x_v, x_p) dx_v \quad (3)$$

$$= \sum_{kl} a_{ik}^*(x_p) v_{kl}(x_p) a_{jl}(x_p). \quad (4)$$

V_{00} and V_{0j} are pseudopotentials which give the elastic and inelastic scattering more correctly than the original potentials v_{00} and v_{0j} .

3. Upper Limits on Scattering Cross Sections

We now show that the improved treatment above can lead to upper limits on scattering cross sections, firstly by considering the simple case of a target system with a valence particle assumed to have only two states.

If the ground state has an unperturbed energy E_0 and the excited state is E_1 , the unitary transformation (1) is (Davydov 1965)

$$\Psi_0 = \psi_0 \cos \frac{1}{2}\beta - \psi_1 \sin \frac{1}{2}\beta, \quad \Psi_1 = \psi_0 \sin \frac{1}{2}\beta + \psi_1 \cos \frac{1}{2}\beta, \quad (5, 6)$$

where

$$\tan \beta = v_{01}/\frac{1}{2}(E_1 + v_{11} - E_0 - v_{00}). \quad (7)$$

The transition potential effective in inelastic scattering is then, from equation (4),

$$V_{01} = v_{01} \cos \beta + \frac{1}{2}(v_{00} - v_{11}) \sin \beta. \quad (8)$$

As $v_{01} \rightarrow 0$,

$$V_{01} \rightarrow v_{01} + (v_{00} v_{01} - v_{01} v_{11}) / (E_1 + v_{11} - E_0 - v_{00}), \quad (9)$$

so that V_{01} is proportional to v_{01} for small v_{01} , as expected from first-order perturbation theory. The second term on the right of the limit (9) is the polarization potential, and is a second-order term corresponding to an elastic collision followed by an inelastic collision or vice versa. As v_{01} increases, V_{01} approaches a limiting value which is, from equation (8) with (7),

$$V_{01}^{\max} = \frac{1}{2}(E_1 - E_0). \quad (10)$$

We thus have a limit on the transition potential effective in inelastic scattering and hence on the inelastic cross section σ_{in} . Assuming the limiting value of V_{01} is

reached within the nuclear radius a and substituting in the plane wave Born approximation, we find that σ_{in} is appreciably less than $(2l+1)(k_x a)^4/k^2$ for the first few values of l , where $k_x^2 = E_1 - E_0$ is taken to be the energy of the strongest excitation of the nucleus and k^2 is the projectile energy. Usually $k_x a$ is less than unity, and then we may write $\sigma_{in} < (2l+1)/k^2$. This value is to be compared with the limiting value $(2l+1)\pi/k^2$ set by consideration of particle flux (Mott and Massey 1965), which is reached asymptotically with increasing values of v_{01} in a simple model employing strong coupling between two channels (Massey and Mohr 1937).

The limit set by channel coupling arises from the unitarity of the S -matrix and is an overall limit. The limit set by the polarized orbital method arises from the unitarity of the matrix transformation (1), and is more stringent, being connected with only one of the physical processes in the collision.

4. Overestimation of Effect of Core Polarization by Perturbation Theory

We now suppose that the target system has three bound states 0, 1 and 2, and consider excitations from state 0 to state 1, either directly or by virtual transitions through the intermediate state 2.

The probability of the two-stage process may be comparable with that of the direct process if the couplings to the intermediate state are strong, as for a collective state, and this is the basis of the core polarization model (Love and Satchler 1967), in which the intermediate state is an excited state of the core and the final state has an excited valence particle and de-excited core. We first take the intermediate state to be an excited state of the valence particle.

We are interested in the effective transition potential V_{01} as expressed in terms of the v_{kl} of equation (4). The three diagonal matrix elements v_{00} , v_{11} and v_{22} as functions of x_p will generally be peaked near the nuclear surface and be of similar form. If we take them to be of identical form, the sum of the three diagonal terms in the expression (4) for V_{01} becomes

$$v_{00} \sum_k a_{0k}^* a_{k1} = v_{00} \langle \Psi_0 | \Psi_1 \rangle = 0.$$

We therefore neglect these three terms so that we can concentrate on the dependence of V_{01} on the three off-diagonal elements v_{01} , v_{02} and v_{21} .

To find the a_{ik} in equation (4) requires the diagonalization of a 3×3 matrix, and this can only be carried out numerically, giving little insight into the problem. We therefore consider the typical case where the transition through the intermediate state is of the same strength as the direct transition, and see what relation this implies between the three transition potentials in perturbation theory. The latter gives

$$a_{ik} = 1, \quad k = i, \quad (11a)$$

$$= v_{ki}/(E_i - E_k), \quad k \neq i, \quad (11b)$$

which we substitute in equation (4). If we neglect the three terms of third order in the v_{ki} , we have

$$V_{01} = v_{01} - v_{02} v_{21} \{ (E_2 - E_1)^{-1} + (E_2 - E_0)^{-1} \}. \quad (12)$$

The first-order term v_{01} corresponds to the direct transition and the second-order

term in $v_{02} v_{21}$ to the transition through an intermediate state. The two corresponding scattering amplitudes add if $E_2 > E_1$ and the v_{kl} are negative. In the diagonalization method, we have $(a_{00} a_{11} + a_{01} a_{10}) v_{01}$ for the direct term and corresponding terms in v_{02} and v_{21} in equation (4) for the virtual transitions, where the a_{ik} are no longer given by the relations (11).

We now take the intermediate state to be an excited state of the core. Let superscripts p, v and c refer respectively to the projectile, valence particle and core particle (or collective state of the core), and let ψ_0 and ψ_1 denote the ground and excited state of the valence particle, and χ_0 and χ_1 similarly for the core. Then the initial, intermediate and final states of the target system are $|0\rangle = \chi_0 \psi_0$, $|2\rangle = \chi_1 \psi_0$ and $|1\rangle = \chi_0 \psi_1$ respectively. The total potential energy of the system is $v = v^{pv} + v^{pc} + v^{cv}$, and so the transition potentials $v_{ij}(x^p) \equiv \langle i|v|j\rangle$ acting on the projectile at the point x^p contain in their component terms the quantities:

$$\begin{aligned} v_{ij}^{pv} &= \int \psi_i^* v^{pv} \psi_j dx^v, \\ v_{ij}^{pc} &= \int \chi_i^* v^{pc} \chi_j dx^c, \\ v_{ik,jl}^{cv} &= \iint \chi_i^* \psi_j^* v^{cv} \chi_k \psi_l dx^c dx^v. \end{aligned}$$

Integrating over all x^c and x^v and using the orthonormal properties of the ψ 's and χ 's gives, to second order,

$$\begin{aligned} V_{01} &= \langle 0|v|1\rangle - \langle 0|v|2\rangle G \langle 2|v|1\rangle \\ &= (v_{01}^{pv} + v_{00,01}^{cv}) - (v_{01}^{pc} G v_{01,01}^{cv} + v_{01,00}^{cv} G v_{01,01}^{cv}). \end{aligned}$$

The second term in each parenthesis is independent of x^p and therefore does not contribute to the scattering. So, as far as the scattering is concerned, we have the term v^{pv} for the direct transition (referred to as D) and the term $v^{pc} G v^{cv}$ for the core polarization (referred to as C). As these terms are functions of the projectile coordinates only, it is immaterial for our purpose whether the intermediate state involves the excitation of valence particles or core particles, or whether the core states are single-particle or collective. We can still label the two terms v_{01} and $v_{02} G v_{21}$ respectively.

Core polarization calculations often do not state the numerical values of the parameters used. However, the paper by Love and Satchler (1967) shows, for the 1.98 MeV level in ^{18}O , the two form factors C and D having similar radial distributions, with maximum values near the nuclear surface of about the same magnitude as the excitation energy. Specimen values of the parameters were therefore selected to make the two terms C and D in equation (12) of equal magnitude. For chosen values of the energy denominators and the ratio v_{02}/v_{21} , the values of v_{02} and v_{21} were determined in terms of v_{01} . Typical sets of values were chosen to give the results shown in Fig. 1 for various values of the determining parameter v_{01} (the quantities are in arbitrary units of energy). The curves labelled P are for the two terms C and D as given by perturbation theory. The curves labelled C and D show the

values of the indirect and direct transition potentials obtained by diagonalizing the energy matrix and substituting the eigenvector components a_{ik} into equation (4).

Perturbation theory is seen to become increasingly inadequate with increasing values of v_{01} , not only in seriously overestimating the magnitudes of C and D , but also in respect of their ratio. For $v_{12} = v_{02}$, the values of C and D attain maximum

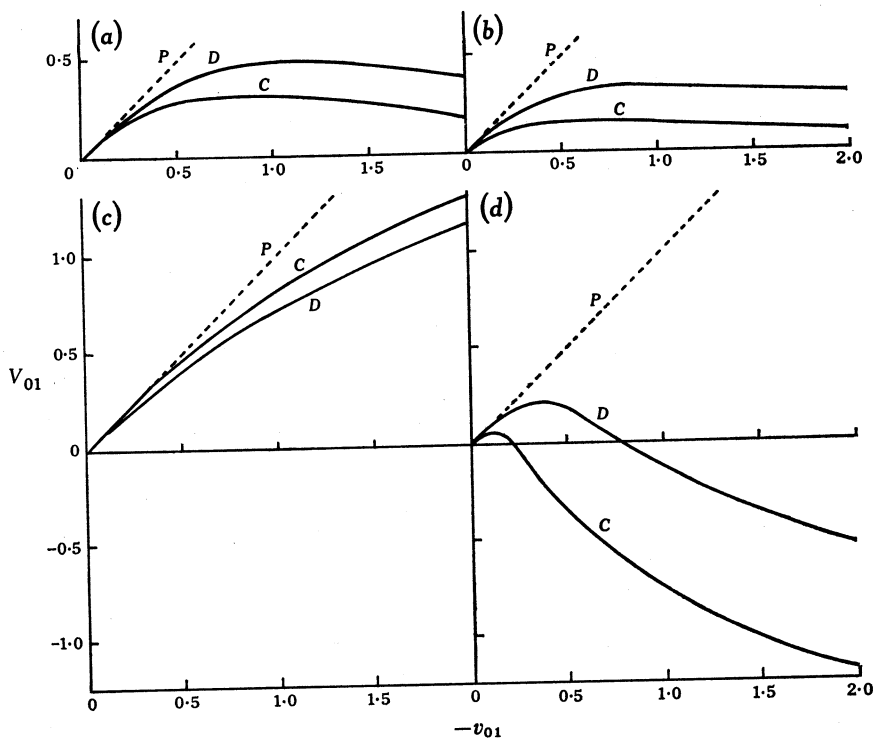


Fig. 1. Illustrating the effective potential V_{01} for transitions from state 0 to state 1 of the target system as a function of the direct transition potential v_{01} . Curve D shows the contribution from direct transitions and curve C the contribution from virtual transitions through an intermediate state 2, calculated by diagonalization of the energy matrix. The transition potentials v_{02} and v_{12} were fixed in terms of v_{01} by choosing their ratio and making the contributions D and C equal in the perturbation theory formula (12). The perturbation theory result for the two contributions is shown by the dashed line P . All quantities are in arbitrary units of energy. The values of the parameters are:

	(a)	(b)	(c)	(d)
$E_1 - E_0$	1	1	1	1
$E_2 - E_0$	2	1.2	2	2
v_{02}/v_{12}	1	1	4	$\frac{1}{4}$

values surprisingly soon, with a ratio of about two over nearly the whole range instead of the ratio of unity given by perturbation theory. The curves for the smaller energy denominators have lower maxima as might be expected from equation (7): one may not boost the term C just by taking a small energy denominator. For $v_{02} > v_{12}$ the discrepancies are less, while for $v_{02} < v_{12}$ they are greater, the actual signs being reversed for the greater values of v_{01} , so that perturbation theory is completely misleading for all but the smallest values of these quantities.

For radial distances appreciably greater or less than the nuclear radius, C and D will be small in magnitude compared with the excitation energy, and so will be given well enough by perturbation theory. For protons on heavy nuclei, perturbation theory may be satisfactory: thus for the 4.07 MeV level in ^{208}Pb , Love and Satchler (1967) find maximum values of C and D of about one-tenth the excitation energy. The overall inaccuracy of perturbation theory values can be determined only by detailed calculation in a given case.

5. Reduction of Polarization Potential by Dynamic Effect

The general treatment of polarization, including that of Section 2 above, is based on the static approximation, which assumes that the energy of the projectile is low enough for its transit time past the target system to be long compared with the orbiting times of the target particles. At higher energies the target system has time to respond only partially to the field of the projectile, and the polarization potential is reduced.

Garrett (1969) has obtained and applied equations for dynamic distortion for the elastic scattering of low energy electrons and positrons by hydrogen atoms. His curves show that the polarization potential, at the distances at which it is largest, is reduced to about 0.8 of the static value for an incident energy of 0.09 Ry, and to about 0.6 of the static value for an incident energy of 0.25 Ry. Remembering that the energy of the first excited state of the atom $E_1 - E_0$ is 0.75 Ry, one may wonder how much further the polarization potential will be reduced for energies above excitation. The core polarization model is used for incident energies which are several times the excitation energy.

Using a simple nuclear model and a δ -function interaction between nucleons, we find that the polarization potential decreases most rapidly as k^2 increases from zero towards the excitation energy and then tends slowly towards a limiting value as k^2 becomes large. This last point is understandable, for when the transit time of the projectile is already short compared with the orbiting times of the target particles, any further reduction in transit time will produce little further decrease in the response of the target system to the field of the projectile. As k^2 is increased from small to large values, the reduction in the polarization potential is to about 0.5 of its static value for a light nucleus ($A \sim 18$) and to about 0.8 for a heavy nucleus ($A \sim 200$). For inelastic collisions we might expect the reduction to be about the same when k^2 is appreciably greater than $E_2 - E_0$ and $E_2 - E_1$.

The preceding remarks are also relevant to the core polarization model in view of the formalism in the previous section. It appears, therefore, that much of the effect which the model was introduced to account for, namely to increase $\sigma_{\text{in}}/\sigma_{\text{e1}}$ (see Section 1), is lost through the dynamic effect alone. Furthermore, it seems to have been overlooked that polarization increases σ_{e1} as well as σ_{in} , and this fact reduces the value of the model still further.

6. Need for Inclusion of Channel Coupling

In the above treatment the terms C and D are both real, but recent experimental evidence (e.g. Schaeffer and Glendinning 1973) indicates that D contains a complex phase factor. A theoretical basis for this is provided by the channel coupling

formalism. Channel coupling involves virtual transitions between different projectile channels, and this is complementary to target polarization with its virtual transitions between different target states; the same v_{ij} are involved.

We consider the modified radial wavefunctions for the projectile F_0 , F_1 and F_2 in the three channels, coupled together by the potentials v_{01} , v_{02} and v_{12} . These potentials are taken to be real as before, and to be monopole for simplicity, so that only partial waves of the same order l are coupled together. The three coupled differential equations have three independent regular solutions for each l which can be taken to have the following asymptotic forms:

Channel	Solution I	Solution II	Solution III
0	$\sin(\rho_0 + \delta_0)$	$g_0 \sin(\rho_0 + \eta_0)$	$h_0 \sin(\rho_0 + \phi_0)$
1	$f_1 \sin(\rho_1 + \delta_1)$	$\sin(\rho_1 + \eta_1)$	$h_1 \sin(\rho_1 + \phi_1)$
2	$f_2 \sin(\rho_2 + \delta_2)$	$g_2 \sin(\rho_2 + \eta_2)$	$\sin(\rho_2 + \phi_2)$

where

$$\rho_0 = k_0 r - \frac{1}{2}l\pi, \quad \rho_1 = k_1 r - \frac{1}{2}l\pi, \quad \rho_2 = k_2 r - \frac{1}{2}l\pi.$$

Thus we suppose solution I is obtained by starting off with F_0 as given by the first of the coupled equations with v_{01} , v_{02} , F_1 and F_2 zero, then slowly turning on v_{01} and v_{02} to produce finite F_1 and F_2 and modifications to F_0 ; similarly for solutions II and III. For small v_{ij} we therefore expect the proportionalities:

$$f_1 \propto v_{01}, \quad f_2 \propto v_{02}, \quad g_2 \propto v_{12}, \quad h_1 \propto v_{21}. \quad (13)$$

The general asymptotic solution for each channel is a linear combination of the three solutions, with coefficients a , b and c , say, and has to be equated to the corresponding general asymptotic form when channel 0 is the entrance channel:

$$F_0 \sim \sin \rho_0 + \alpha_0 \exp i\rho_0, \quad F_1 \sim \beta_1 \exp i\rho_1, \quad F_2 \sim \beta_2 \exp i\rho_2,$$

where $|\alpha_0|^2$ is the probability of elastic scattering and $k_1 k_0^{-1} |\beta_1|^2$ and $k_2 k_0^{-1} |\beta_2|^2$ the probabilities for inelastic scattering into exit channels 1 and 2 respectively. Fitting the general solutions to the asymptotic forms and also fitting their slopes gives six simultaneous equations for the six unknowns a , b , c , α_0 , β_1 and β_2 . Each of the quantities α_0 , β_1 and β_2 may be expressed in terms of the quotient of two determinants; the determinant in the denominator in each case is the same and is of no particular significance for us here. We are interested in β_1 , and for this quantity the determinant in the numerator is found, on reduction, to contain the terms

$$f_1 \sin(\delta_1 - \eta_1) \exp(-i\phi_2) + f_2 h_1 \sin(\eta_1 - \phi_1) \exp(-i\delta_2) \\ + f_1 g_2 h_1 \sin(\phi_1 - \delta_1) \exp(-i\eta_2). \quad (14)$$

If we replace the factors f , g and h by the corresponding v_{ij} according to the relations (13), the three terms in (14) have as coefficients v_{01} , $v_{02} v_{21}$ and $v_{01} v_{12} v_{21}$ respectively, and so are identified as first-order, second-order and third-order terms respectively. The determinant in the denominator for β_1 contains a term of zero order in v_{ij} . We now note that there is a phase difference $\delta_2 - \phi_2$ between the first-order and second-order terms, and $\eta_2 - \phi_2$ between the first-order and third-order terms.

When the projectile is incident with the threshold energy E_2 for the two-stage process, it emerges in channel 2 with zero energy, and then ϕ_2 , δ_2 and η_2 are integral multiples of π , so that the first-order, second-order and third-order terms are all in phase. As the projectile energy increases, the terms get increasingly out of phase.

Polarization may be taken into account in the above formalism by replacing the v_{ik} by the V_{ik} of Section 2, and this should be done, for we may expect the effects of polarization and channel coupling to be of comparable magnitude. This last point has been confirmed for the simpler case of elastic scattering with only two channels, taking square wells of various depths. The change in zero-order phase shift produced by channel coupling has an imaginary component which increases from zero at the excitation energy to a value comparable in magnitude with the real component at twice the excitation energy, at which energy the (real) change in phase shift produced by polarization is of comparable (and slightly greater) magnitude.

In short, we should use the pseudopotentials V_{ij} in the coupled equations, not just in the distorted wave Born approximation.

7. Conclusions

The usual treatment of core polarization cannot be relied upon to give more than the magnitude of its effect. To obtain more reliable results one should use matrix diagonalization in place of perturbation theory, and take account of dynamic effects and channel coupling.

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Manuscript received 19 September 1974