01 Oct 1981

Orientation of Atoms Excited by Charged Particles at High Impact Energies

Don H. Madison
Missouri University of Science and Technology, madison@mst.edu

Kieth H. Winters

Recommended Citation

D. H. Madison and K. H. Winters, "Orientation of Atoms Excited by Charged Particles at High Impact Energies," *Physical Review Letters*, vol. 47, no. 26, pp. 1885-1887, American Physical Society (APS), Oct 1981.

The definitive version is available at https://doi.org/10.1103/PhysRevLett.47.1885

Orientation of Atoms Excited by Charged Particles at High Impact Energies

D. H. Madison
Department of Physics, Drake University, Des Moines, Iowa 50311

and

K. H. Winters
Theoretical Physics Division, Atomic Energy Research Establishment Harwell, Didcot, Oxon OX11 0RA, England
(Received 13 October 1981)

A perturbation-expansion approach is used to examine the sign of the orientation vector as a function of scattering angle and projectile charge. It is shown that for small angles, the sign of the orientation vector is different for oppositely charged projectiles consistent with the prediction of the classical grazing model. At large angles, on the other hand, the orientation vector for oppositely charged projectiles is shown to have the same sign.

PACS numbers: 34.80.Dp

Recent experiments of electron-impact excitation have revealed that the target atoms can become strongly oriented during the collision process. This orientation results from the transfer of projectile orbital angular momentum to target angular momentum. The early e-He experiments (Eminyan *et al.*[1,2]) determined the magnitude of the orientation vector but not the sign. Later, Standage and Kleinpoppen[3] showed that the sign was positive at small angles for e-He scattering. This sign is consistent with a classical grazing model which would predict a positive orientation for attractive collisions and a negative orientation for repulsive collisions. The quantum-mechanical distorted-wave calculation of Madison and Shelton[4] also predicted a positive orientation for the e-He problem but the physics responsible for this sign was not clear because of the many multiple summations.

Over the last few years, there has been considerable interest in understanding the sign of the orientation vector. Recently, Kohmoto and Fano[5] have related the sign of the orientation vector to the sign of phase differences between elements of the transition matrix. They argue that sign reversal of the projectile charge reverses the signs of the phases which in turn reverses the sign of $O_{1-}{}^{c}$. Using a similar approach, Hermann and Hertel[6] have related the quantum-mechanical results to the predictions for a classical grazing collision at small scattering angles. In both of these works, the quantum-mechanical amplitudes were evaluated using partial-wave expansions which eventually resulted in multiple summations from which information about the sign of the orientation vector was extracted. Here, we point out a problem with this approach and show that the relative sign of the orientation vector for oppositely charged projectiles can be quickly predicted for small- and large-angle scattering from well-known properties of the various terms in the Born series.

The effect on the scattering amplitude of changing the sign of the projectile charge is most easily seen in a perturbation approach. This restricts us to the case of impact at high energies, where the Born series is expected to converge. The Born expansion of the T matrix $T_{ba}{}^{q}$ for the transition $a \to b$ of the target, induced by impact of a projectile of charge q, is (neglecting exchange)

$$T_{ba}{}^{q} = \langle \Phi_b | V | \Phi_a \rangle + \langle \Phi_b | V G_0{}^{(+)} V | \Phi_a \rangle + \dots , \tag{1}$$

where $|\Phi_{a,b}\rangle$ are the asymptotic states in the initial and final channels, V is the projectile-target interaction, and $G_0{}^{(+)}$ is the free-particle Green's function with outgoing-wave boundary conditions. Equation (1) may be written as

$$T_{ba}{}^{q} = q t_{ba}{}^{1} + q^2 t_{ba}{}^{2} + \dots , \tag{2}$$

where the terms $t_{ba}{}^{n}$ are complex functions of energy and momentum transfer (except for $n = 1$) and are independent of q. The terms on the right-hand side of Eq. (2) are, of course, the first and second Born contributions to the T matrix.

For the particular case of positron impact ($q = +1$ in atomic units) we have, trivially,

$$T_{ba}{}^{+1} = t_{ba}{}^{1} + t_{ba}{}^{2} + \dots$$

while for electron impact ($q = -1$) we have

$$T_{ba}{}^{-1} = -t_{ba}{}^{1} + t_{ba}{}^{2} + \dots .$$

Now we know from the work of several authors (e.g., Potapov[7]) that in the high-energy large-momentum-transfer limit the Born series converges to its second term $q^2 t^2$ in the case of excitation, and hence we have that

$$T_{ba}^{+1} = T_{ba}^{-1}$$

in this limit. It follows that the sign of the orientation vector must then be the same for electron and positron impact.

In contrast to this, at small momentum transfers and high energies the Born series is dominated by the first term which exhibits a charge sign dependence. This sign difference for $q = \pm 1$ should be observable in quantities such as the orientation vector which depends upon the complex nature of the amplitudes. This can be seen as follows. Consider an atom which has been excited by charged particle impact such that the final atomic state may be written (neglecting spin for simplicity)

$$|\psi_f\rangle = \sum_{m_b} T_{m_b}{}^q |m_b\rangle , \tag{3}$$

where $|m_b\rangle$ represents an atomic wave function of orbital angular momentum L and projection m_b. The expectation value for the angular momentum of the atom perpendicular to the scattering plane is then (y direction is $\vec{p}_i \times \vec{p}_f$)

$$\langle L_y\rangle = (i\hbar/2) \sum_{m_b} T_{m_b}{}^q [T_{m_b-1}{}^{q*} A_{m_b}{}^- - T_{m_b+1}{}^{q*} A_{m_b}{}^+] , \tag{4}$$

where

$$A_{m_b}{}^+ = [(L - m_b)(L + m_b + 1)]^{1/2}$$

and

$$A_{m_b}{}^- = [(L + m_b)(L - m_b + 1)]^{1/2}.$$

For atomic states with $L = 1$ and $T_{-1}{}^q = -T_{+1}{}^q$,

$$\langle L_y\rangle = -2\sqrt{2}\,\hbar\,\mathrm{Im}(T_0{}^{q*} T_1{}^q) . \tag{5}$$

If the expansion (2) converges to the first two terms, for $L = 1$

$$\langle L_y\rangle = -2\sqrt{2}\,\hbar\,\mathrm{Im}[t_0{}^{1*} t_1{}^1 + q(t_0{}^{1*} t_1{}^2 + t_0{}^{2*} t_1{}^1 + t_0{}^{2*} t_1{}^2] . \tag{6}$$

However, the first term in the above expression is the first Born approximation for the orientation vector which vanishes. Consequently,

$$\langle L_y\rangle = 2\sqrt{2}\,\hbar\,\mathrm{Im}[q(t_0{}^{1*} t_1{}^2 + t_0{}^{2*} t_1{}^1) + t_0{}^{2*} t_1{}^2] . \tag{7}$$

Examination of Eq. (7) reveals that if $t^1 \gg t^2$, there should be a charge-dependent sign difference for the orientation vector and if $t^2 \gg t^1$, there will be no charge dependence. Consequently, one would expect opposite signs for the orientation vector at small angles for e^- and e^+ scattering, and the same sign at large angles. It should be noted that this conclusion results from the vanishing of the first Born approximation to $\langle L_y\rangle$. We cannot predict at the present which projectile will exhibit the sign reversal, nor the sign at large angles, except by explicit computation of the orientation vector in an appropriate approximation.

At this point it is interesting to compare our results with the conclusions of Kohmoto and Fano.[5] Their analysis relates the sign of the orientation vector to the complex phases of the T matrix. Using a partial wave expansion, the T matrix may be expressed as

$$T_{ba}{}^q = \sum_\mu B_\mu{}^q \exp(i\varphi_\mu) , \tag{8}$$

where μ represents the appropriate collective angular momentum quantum numbers. In the distorted-wave or similar approximations, φ_μ may be expressed as the sum of the ordinary phase shifts for the individual distorted waves. In this case the arguments of Kohmoto and Fano[5] suggest that changing the sign of the projectile will change the sign of the orientation vector since the partial-wave phase shifts will change signs for the small-order partial waves. This argument will be valid if $B_\mu{}^q B_{\mu'}{}^q$ has the same sign as $B_\mu{}^{-q} B_{\mu'}{}^{-q}$ for all $\mu\mu'$. However, we would like to point out that with the above phase choice, $B_\mu{}^q$ can be either positive or negative contrary to Eq. (11n) of Kohmoto and Fano[5] or Eq. (3) of Hermann and

Hertel.[6] The sign of $B_\mu{}^q$ will depend upon an integral involving initial- and final-state partial waves and a potential. Since this sign will depend strongly on the details of the contributing distorted waves, there is no guarantee that the above relationship will hold. Examination of these integrals for excitation of helium by electrons and positrons revealed that for various μ the above relationship was often valid but that the exceptions were significant.

The relationship between the present analysis and the distorted-wave approximation may be understood as follows. If the distorted-wave approximation is expanded in terms of the Born series, one finds that the first-order distorted-wave term contains the first Born term, parts of the second Born term which are important for large-angle scattering, and higher-order Born terms. Consequently, the predictions of the present second-order model should be observed in a first-order distorted-wave calculation since they both contain the important physics of the Born series.

We now look at the results of a computation of $O_{1^-}{}^c$ for the specific case of excitation of He($2\,{}^1P$) from the ground state by both electron and positron impact at an energy of 100 eV. The calculation is a second-order distorted-wave approximation including first-order exchange (electron scattering), which generalizes the second-order distorted-wave Born-approximation model of Winters[8] to the case of $s \rightarrow p$ transitions. The details of the second-order Born-approximation calculation which forms a part of this model are similar to those of Joachain and Winters,[9] except that here we include the central parts of the $1\,{}^1S$ and $2\,{}^1P$ state contributions exactly while the other intermediate states are computed with an average excitation energy of 1.8 Ry. The results of the calculation are presented in Fig. 1. Examination of this figure reveals the predicted sign reversal for small angles and identical signs for large angles. In this case the electron scattering results change sign between small and large angles. The fact that the large-angle results are almost identical stems from the choice for the average excitation energy. A careful examination of the second-order distorted-wave approximation will be presented in a later publication.

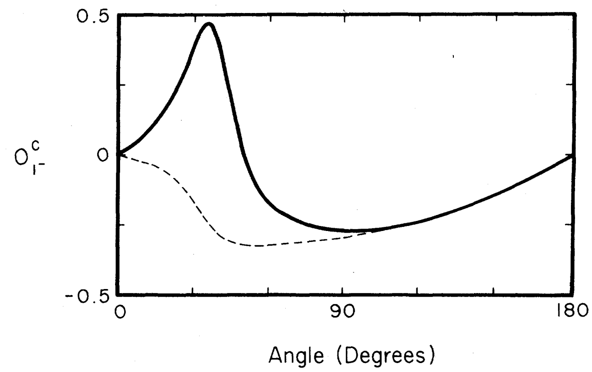

FIG. 1. Orientation vector for excitation of the $2\,{}^1P$ state of helium by 100-eV electrons (solid curve) and positrons (dashed curve) as a function of projectile scattering angle. The theoretical curves are second-order distorted-wave calculations.

This work was supported in part by a Northwest Area Foundation Grant of the Research Corporation.

[1] M. Eminyan, K. B. MacAdam, J. Slevin, and H. Kleinpoppen, Phys. Rev. Lett. 31, 576 (1973).

[2] M. Eminyan, K. B. MacAdam, J. Slevin, and H. Kleinpoppen, J. Phys. B 7, 1519 (1974).

[3] M. C. Standage and H. Kleinpoppen, Phys. Rev. Lett. 36, 577 (1976).

[4] D. H. Madison and W. N. Shelton, Phys. Rev. A 7, 499 (1973).

[5] M. Kohmoto and U. Fano, J. Phys. B 14, L447 (1981).

[6] H. W. Hermann and I. V. Hertel, J. Phys. B 13, 4285 (1980).

[7] V. S. Potapov, Zh. Eksp. Teor. Fiz. 63, 2094 (1973) [Sov. Phys. JETP 36, 1105 (1973)].

[8] K. H. Winters, J. Phys. B 11, 149 (1978).

[9] C. J. Joachain and K. H. Winters, J. Phys. B 10, L727 (1977).