Vacuum polarization- and molecular-potential effects in heavy-ion scattering*

Johann Rafelski
Argonne National Laboratory, Argonne, Illinois 60439
(Received 18 February 1975; revised manuscript received 3 November 1975)

The corrections to the heavy-ion scattering cross sections due to the presence of perturbing vacuum polarization and molecular potentials are evaluated. We find effects on the cross section up to 0.7% in ^{16}O with ^{208}Pb collisions due to vacuum polarization and up to 2.6% in U with Th collisions due to molecular and vacuum polarization corrections.

[NUCLEAR REACTIONS Calculations of modifications of elastic heavy-ion $\sigma(\theta)$ due to vacuum polarization and molecular potentials.]

Large angle ($\theta_{c.m.} > 10°$) heavy-ion scattering is mainly determined by Coulomb, and above the Coulomb barrier by nuclear forces. However, with increasing precision of the experiments it might be possible to measure the deviation from pure Coulomb scattering at sub-Coulomb barrier energies due to vacuum polarization and molecular effects. The former effect has been a recent matter of interest[1,2] and we aim in this note at a clarification of the possible experimental consequences. The latter effect due to the molecular potential[3] is most important for collisions with $Z = Z_{\text{projectile}} + Z_{\text{target}} \gtrsim 130$. Its origin is from the quasimolecular electrons that are bound to the combined system of projectile and target nucleus. The relative importance of the molecular potential V_{mol} as compared with the Coulomb potential of the nuclei depends heavily on the combined charge Z of projectile and target in the relativistic domain. For collisions with $(Z_1 + Z_2) \sim 184$ the molecular potential reaches -6.2 MeV at $R = 15$ fm, which is about 0.8% of the Coulomb barrier.

The method used in this note for calculating corrections to heavy-ion cross sections is the classical approximation. The heavy ions are assumed to move on classical trajectories in a given potential. The well-known solution of the Newtonian equations of motion will not be reviewed here—but some practical points pertaining to the numerical problem are mentioned. Consider the scattering of two particles interacting via a Coulomb potential V perturbed by a small additional interaction δV:

(a) Numerically, it turned out that direct calculation of the influence of an additional potential δV on the cross section is more practical than a perturbation expansion in $\delta V/V$.

(b) To obtain the classical cross section in the vicinity of a scattering angle θ_C the value of the corresponding Coulomb angular momentum L_C is used:

$$L_C = \alpha Z_1 Z_2 (\mu/2T)^{1/2} \cot(\tfrac{1}{2}\theta_C) \tag{1}$$

(μ is the reduced mass, $T = m_2/(m_1+m_2)E$, E is the lab projectile energy, and α is the fine structure constant.)

(c) The scattering angle corresponding to a given L_C (or equivalent, to a given impact parameter) is obtained from

$$\tfrac{1}{2}(\pi - \theta) = \int_{R_{\min}(L_C)}^{\infty} \frac{L_C}{r^2\{2m[E - V(r)] - L_C^2/r^2\}^{1/2}}\, dr, \tag{2}$$

where the distance of closest approach $R_{\min}$ corresponds to the only zero of the square root in the repulsive, monotone, ion-ion potential. It is found numerically for any $V(r)$.

(d) The numerical integration in Eq. (2) is cut off at a suitable value $\tilde{R} = R_{\min} + \delta$ to avoid the $1/(r - R_{\min})^{1/2}$ singularity. The remaining part is approximately evaluated analytically ($\partial V/\partial r$ is needed).

(e) The cross section is finally calculated from

$$\frac{d\sigma(\theta)}{d\Omega} = L_C(\theta) \frac{\partial L_C(\theta)}{\partial \theta} \Big/ (m^2 v^2 \sin\theta), \tag{3}$$

where we now consider $d\sigma/d\Omega$ to be the function of the calculated angle θ [Eq. (2)]. $\partial L_C/\partial\theta$ is obtained differentiating Eq. (2) with respect to θ. Again the cut-off method as mentioned in (d) is employed. To maintain the appropriate accuracy we need to know $(\partial^2 V/\partial r^2)/R_{\min}$.

(f) The above procedure gives us the cross section at an angle $\theta = \theta_C + \Delta\theta$. The cross section at the point θ_C is then obtained from the Taylor expansion around θ_C:

$$\left.\frac{d\sigma}{d\Omega}\right|_{\theta_C} = \left.\frac{d\sigma_R}{d\Omega}\right|_{\theta_C} + \delta \left.\frac{d\sigma_R}{d\Omega}\right|_{\theta_C}$$

$$= \left.\frac{d\sigma_R}{d\Omega}\right|_{\theta_C+\Delta\theta} - \Delta\theta \frac{\partial}{\partial\theta}\left.\frac{d\sigma_R}{d\Omega}\right|_{\theta_C}$$

$$+ \delta \left.\frac{d\sigma_R}{d\Omega}\right|_{\theta_C+\Delta\theta} - \Delta\theta \frac{\partial}{\partial\theta}\delta \left.\frac{d\sigma_R}{d\Omega}\right|_{\theta_C} + \mathcal{O}[(\Delta\theta)^2]$$

and therefore

$$\left.\frac{d\sigma}{d\Omega}\right|_{\theta_C} = \left.\frac{d\sigma}{d\Omega}\right|_{\theta_C+\Delta\theta} - \Delta\theta \frac{\partial}{\partial\theta}\left.\frac{d\sigma_R}{d\Omega}\right|_{\theta_C} + \mathcal{O}[(\delta\theta)^2], \quad (4)$$

where the subscript R stands for "Rutherford."

(g) Numerical tests for precision have shown that the outlined procedure has sufficient accuracy to calculate effects of the order of 0.01% of the total Coulomb cross section after the numerical error has been minimized by variation of the number of integration points, their distribution, and the cut-off value δ. In particular we have used $r = R_{\min}/t$, $t \in (0, 1)$, and $\delta = 1.7\times10^{-4} R_{\min}$, and we have found 2000 points of integration to be necessary in (c) and (e). In the tests we have used a small $1/r$ term (of the order of 1% of V) as a perturbing potential.

The classical approximation can be used for an asymmetric collision whenever the scattering parameter $\eta \gg 1$ ($\eta = Z_1 Z_2 \alpha c/v_\infty$). However, even in collisions of identical nuclei, where $\eta \gtrsim 500$ (say U, Th at 1.6 GeV), the oscillations of the cross section would be averaged in any practical counter—therefore, our approach is valid also in this case.

Vacuum polarization in heavy-ion scattering has been first considered in Ref. 1. Among other results it was found that with increasing momentum transfer $\vec{q}$ between the heavy ions the quantity defined by

$$\frac{d\sigma}{d\Omega}\Big/\frac{d\sigma_R}{d\Omega} = 1 + \epsilon \quad (5)$$

is a rising function of $\vec{q}^2$, $\epsilon \sim \ln(\vec{q}^2)$. Subsequently, Roskies[2] pointed out that the expansion in η which has been used to evaluate the scattering amplitude in Ref. 1 overestimates the effect of the vacuum polarization for large $\vec{q}^2$. The present calculations therefore aim to determine the behavior of ϵ for large $\vec{q}$. Our efforts to calculate this behavior in the frame set by Ref. 1 failed because of particularly pathological behavior of the scattering amplitude for very large η, q^2.

We have evaluated the quantity ϵ defined by Eq. (5), inserting the vacuum polarization potential

$$eV_C + eV_{vp} = (Z_1 Z_2 \alpha/r)\left(1 + 2\alpha/3\pi \int_1^\infty f(t)\exp(-2mrt)dt\right), \quad (6)$$

where

$$f(t) = (t^2-1)^{1/2} t^{-2}[1 + (2t^2)^{-1}] \quad (7)$$

into the code discussed above.

We find that the behavior predicted in Ref. 1 for small q^2 is reproduced; for large $\vec{q}^2$ (large θ) we find a constant ϵ. In particular, consider oxygen projectiles of 69.1 MeV (lab) in O → Pb collisions in Fig. 1(a) for which experimental information is available.[5] In the interval 60°–160° we have a rise of 0.15% which is compatible with the results of Barnett *et al.*[5] Use of lower energy projectiles [Fig. 1(a), 30 MeV ^{16}O] will increase the effect if measured between 20° and 80°, where the relative change in ϵ is 0.3%—similarly we could employ a 16 MeV ^{4}He beam [Fig. 1(a)].

We turn now to the discussion of the molecular-potential effects. The total Hamiltonian for the colliding heavy-ion system can be written as the sum of the electron and nucleon parts:

$$H = H_{el}(\vec{R}, \vec{r}_i) + H_n(\vec{R}), \quad (8)$$

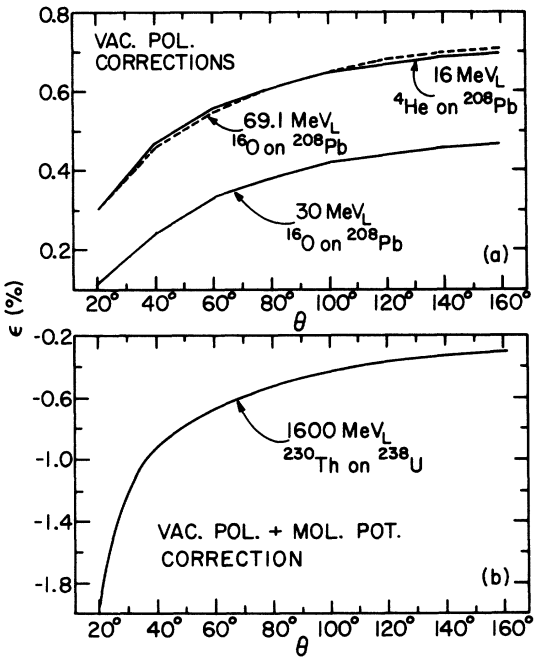

FIG. 1. Correction ϵ to the Rutherford cross section in percent as a function of the lab scattering angle: (a) vacuum polarization corrections in 69.1 and 30 MeV (lab) ^{16}O scattering on ^{208}Pb and (b) vacuum polarization- and molecular-potential correction in 1600 MeV (lab) ^{230}Th scattering on ^{238}U.

where $\vec{R}$ is the distance vector between the heavy ions and $\vec{r}_i$ are the coordinates of the electrons. Using a wave function

$$\psi(\vec{r}, \vec{R}) = \psi_{el}(\vec{r}_i, \vec{R})\psi_n(\vec{R}) \tag{9}$$

and assuming the validity of the adiabatic approximation, the problem of finding $\psi_{el}(\vec{r}_i, \vec{R})$ is reduced to a solution of the relativistic two-center Coulomb potential of the nuclei.[4] The nuclear part of the Hamiltonian reduces to

$$H_{\text{eff } n} = \sum_i [E_i(\vec{R}) - E_i(\infty)] + H_n(\vec{R}), \tag{10}$$

where E_i are the eigenvalue energies of the electrons. Following Ref. 3 we define

$$V_{mol}(\vec{R}) = \sum_i [E_i(\vec{R}) - E_i(\infty)]. \tag{11}$$

The evaluation of the molecular potential, Eq. (11), requires the knowledge of the electronic energy eigenvalues for the relativistic two-center potential.[6] Although the Hartree-Fock calculations describing this potential have not been carried out, an approximate potential originating in the eigenenergies of 28 innermost electrons has been obtained[7] using electron wave functions without electron-electron interactions:

$$V_{mol}(R) = -E_0\left(\frac{R}{r_0}\right)^a e^{-R/r_1}, \quad R > 14.5 \text{ fm}. \tag{12}$$

In the case of U-U (similarly for other large Z scattering systems such as Th–U, etc.) we have

$$E_0 = 3.6 \text{ MeV}, \quad r_0 = 100 \text{ fm}, \quad r_1 = 10\,000 \text{ fm}, \quad \text{and } a = -0.27. \tag{13}$$

Since the mutual shielding of the electrons is not taken account of in the above parameters, it is possible that E_0 is actually smaller by ~15%. [The decrease of E_0 to 3.1 MeV lowers the effects on the cross sections shown in Fig. 1(b) by 15%.] The geometrical structure of V_{mol}, Eq. (12), is not likely to change significantly and has not been varied.

It is not valuable to consider in this connection the collision of identical particles, since the identity of projectile and target will make the cross section symmetric around 45° (lab) preventing a true measurement of backscattering.

As a characteristic example we have therefore chosen the scattering of ^{230}Th on ^{238}U at 1600 MeV (lab). Since the molecular potential is negative[3] and has a magnitude larger than the positive vacuum-polarization potential, we will find a net decrease of the cross section. Furthermore, since the molecular potential grows more slowly than the nuclear Coulomb repulsion, the correction to Rutherford scattering will become smaller with increasing scattering angle. In Fig. 1(b) the results of our calculations are summarized.

We find a change of 1.7% in the cross section as we go from 20° to 160° in scattering angle. This greater change comes because the addition of vacuum polarization and molecular effects enhances the relative effect at chosen scattering angles.

In view of the above calculations we feel that both effects can be well established by measuring heavy-ion differential scattering cross sections. The measurement of the molecular potential will increase our knowledge of the binding of quasi-molecular electrons in very strong external fields.

We would like to thank B. Müller, A. Klein, and J. Schiffer for interesting discussions and L. Goodman and B. Müller for a critical reading of the manuscript.

---

*Work performed under the auspices of the U. S. Energy Research and Development Administration.

[1]J. Rafelski and A. Klein, Phys. Rev. C 9, 1756 (1974).
[2]R. Z. Roskies, Phys. Rev. C 10, 1565 (1974).
[3]J. Rafelski, B. Müller, and W. Greiner, Nuovo Cimento Lett. 4, 469 (1972).
[4]K. Smith, B. Müller and W. Greiner, J. Phys. B 8, 75 (1975).
[5]A. R. Barnett, W. R. Phillips, P. J. A. Buttle, and L. J. B. Goldfarb, Nucl. Phys. A176, 321 (1971).
[6]B. Müller, J. Rafelski, and W. Greiner, Phys. Lett. 47B, 5 (1973); B. Müller and W. Greiner, Z. Naturforsch. 31a, 1 (1976); B. Müller, Ph. D. thesis, Frankfurt/*M*, 1973 (unpublished).
[7]B. Müller (private communication).