the electromagnetic transition rates deviate considerably from those of a triaxial rotor when N is small.

In conclusion, we have suggested a third dynamical symmetry, in addition to SU(5) and SU(3), which may be useful in describing properties of nuclei at the end of major shells. We point out, however, that microscopic calculations in which both proton and neutron bosons are introduced explicitly[9] indicate that the Hamiltonian for the combined system may not be invariant under proton-neutron transformations (the variable called F spin in Ref. 8) at the end of major shells. The O(6) symmetry must then be viewed only as an approximate symmetry describing the main features of the spectra observed at the end of the major shells, and a detailed comparison with experiment may require the explicit introduction of proton and neutron degrees of freedom.

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New Predictions for Rayleigh Scattering: 10 keV–10 MeV

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New theoretical predictions for the contribution to elastic photon scattering from atoms due to the bound atomic electrons are compared with recent experiments and previous theory. At 1.33 MeV, we resolve the large-angle disagreement for experiments on lead. For 2.75-MeV photons scattered by lead, we confirm the theoretical Rayleigh scattering amplitudes of Cornille and Chapdelaine. At 6.84 MeV, we estimate that the form-factor approximation yielded predictions for the L-shell Rayleigh amplitudes which were too large by 15%. For experiments below 100 keV, the form-factor approximation is poor.

We wish to report resolution of discrepancies between theory and several recent experiments[1-7] for high-energy elastic photon scattering, achieved with a new theoretical calculation of the amplitudes for scattering off bound electrons (Rayleigh scattering). At the same time we are able to indicate under what circumstances the form-factor approximation, most commonly used to predict the Rayleigh-scattering amplitudes, is adequate. Subsequently we will present a more systematic discussion of the Rayleigh-scattering amplitudes for all atomic electrons in the keV and MeV range for all atomic numbers. Interest in these Rayleigh amplitudes, important for the determination of absorption coefficients, has also recently arisen in attempts to observe experimentally the Delbrück-scattering amplitudes,[4] from its proposed use[8] as a diagnostic tool for spatial resolution of densities and temperatures of neutrals in plasmas, and because it is a serious background which cannot be distinguished by energy discrimination in nuclear fluorescence experiments.[9]

Our numerical method, expected to be valid for energies from 1 keV to 10 MeV, follows that of Brown and co-workers,[10] which also gives the details of the basic formalism. We assume that the atom is represented by noninteracting electrons in a screened central potential V resulting from the charge distribution of the nucleus and the atomic electrons. Starting with the second-order S-matrix element of the quantum electrodynamic interaction of electrons in an external potential V with radiation, we expand the photon wave functions in multipole series. Electron states and propagators in the atomic potential V are not expanded in V, unlike the Born approximation, but rather the radial functions of a partial-wave series expansion are calculated numerically. We have primarily used the more realistic Dirac-Hartree-Fock-Slater (DHFS) type self-consistent potentials but have also obtained some predictions for the Coulomb potential. For the total atom scattering, we generate the contribution of the lower shells (typically the K, L, and M shells) using the numerical method just described and estimate the small contribution due to the outer shells via the form-factor (or modified-form-factor) approximation. The energy range for which our predictions should be valid is limited at low energies by the neglect of electron-electron correlations and at high energies by excessive computer time requirements to obtain convergent multipole expansions. (At higher energies nuclear-size and -structure effects would also have to be included.)

The discrepancies between theory and experiment occur for medium through heavy atoms in two regions: (1) for photon energies above 1 MeV, and (2) for photon energies below 100 keV. For photon energies intermediate to these two regions, Johnson and Feiock and Cheng and coworkers[11] have recently obtained theoretical predictions in satisfactory agreement with experiment, with which we are in agreement.

In the photon energy range of 0.90–1.33 MeV, Dixon and Storey[1] and other experimenters[2-4] have reported discrepancies between theory and experiment for heavy atoms. For the 1.33-MeV experiments, the disagreement is as much as a factor of 1.8 at large scattering angles. At these energies, the Rayleigh K-shell amplitudes are dominant at most angles; the theoretical amplitudes have been based on a numerical calculation of Brown and Mayers[10] for the K shell of mercury at 1.31 MeV using the Coulomb potential. We have calculated the Rayleigh amplitudes at 1.33 MeV for the K shell of lead using DHFS wave functions, removing the discrepancy between theory and experiments (see Fig. 1). Introducing artificial 3% errors in the dipole terms of our calculations, we obtain errors in the scattering amplitudes whose magnitudes have an angular dependence similar to those of Brown and Mayers. Because of destructive multipole interference at large angles for this high energy, a factor-of-2 error in cross section can result from this seemingly small 3% multipole error.[12] At the same

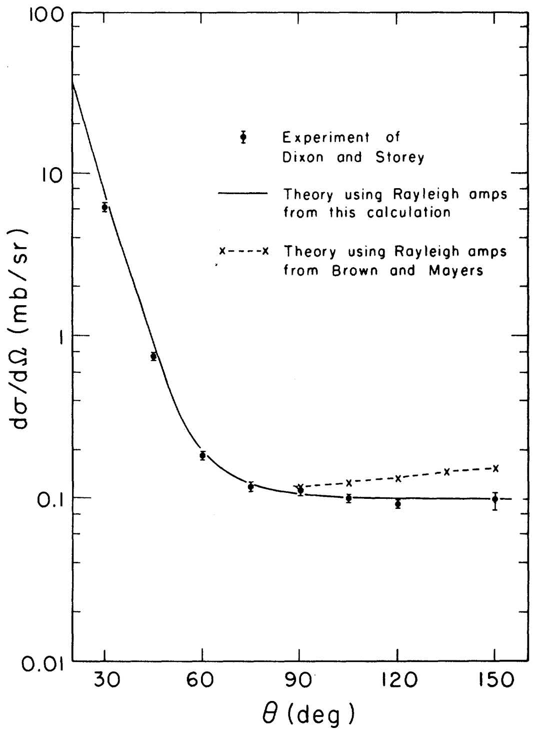

FIG. 1. Differential elastic-photon-scattering cross sections vs scattering angle for 1.33-MeV photons scattered by lead, according to the experiment of Dixon and Storey (Ref. 1), this calculation, and utilizing the earlier results of Brown and Mayers (Ref. 10). For angles less than 90 degrees, both theoretical predictions agree reasonably well with experiment.

time our calculation has removed the similar discrepancies reported at 1.12 and 1.17 MeV which also reflect the use of the incorrect 1.31-MeV theoretical point.

At 2.74 MeV, Schumacher and Stoffregen[5] have measured the elastic-scattering cross section of photons from lead for scattering angles of 15 through 150 degrees. Using theoretical Delbrück amplitudes supplied by Papatzacos and Mork,[13] Rayleigh K-shell amplitudes calculated by Cornille and Chapdelaine[14] for 2.62-MeV photons incident on mercury, and nuclear Thomson amplitudes, Schumacher and Stoffregen found good agreement between theory and experiment at scattering angles of 15, 120, and 150 degrees, but found disagreement by factors of 1.2–1.7 at intermediate angles. Our numerical calculation has confirmed the correctness of the Rayleigh amplitudes used in this comparison, within the errors assumed in the paper. The Rayleigh amplitudes dominate only the forward angle of 15 degrees, where there is no significant disagreement. At the large angles of 120 and 150 degrees where there is also no disagreement, the nuclear Thomson amplitudes dominate. For the intermediate angles of 30–90 degrees, where there is large disagreement, the Delbrück amplitudes of Papatzacos and Mork dominate. This suggests that the disagreement is due to errors in the theoretical Delbrück amplitudes, based on the Coulomb Born-approximation (small-$Z\alpha$) calculation of Papatzacos and Mork, here being used in high-$Z\alpha$ elements with many electrons. Papatzacos and Mork had anticipated that the higher-order Coulomb corrections would be most important in this energy region.

Recent measurements of the elastic-scattering cross sections for photons of energies 6.84–11.39 MeV incident on lead and uranium and scattered through 1.5 degrees have been reported by Kahane, Shahal, and Moreh.[5] Using K-shell Rayleigh amplitudes due to Florescu and Gavrila,[15] higher-shell Rayleigh amplitudes estimated from the relativistic form-factor approximation, and Delbrück amplitudes provided by Papatzacos and Mork, Kahane, Shahal, and Moreh found agreement between theory and experiment at all photon energies except 6.84 MeV. The Rayleigh amplitudes dominate this lowest-energy experiment at 6.84 MeV and it is the L shell which dominates the Rayleigh contribution. For the higher energies, where there is no discrepancy, the K-shell amplitude is beginning to dominate the Rayleigh contribution. For these energies and angles the Delbrück amplitudes never strongly dominate the scattering and it has been argued[13] that the Coulomb corrections to the Delbrück scattering will be smaller than at 2.75 MeV. Full numerical calculations for this case are prohibitive because of the increase in computer time requirements with energy to obtain convergent photon multipole series. However, we have verified that the K-shell amplitudes used at these energies and momentum transfers are appropriate: In comparisons between our numerical amplitudes and high-energy amplitudes, convergence within 1% of the high-energy limit[15] had been obtained by about 3 MeV at this momentum transfer of 7.2 Å^{-1}. For the same reason (satisfactory comparisons with lower-energy predictions), we conclude that it is possible to predict the Rayleigh-scattering amplitudes at 6.84 MeV for this momentum transfer for all shells utilizing the modified–form-factor approximation suggested by Brown and Mayers.[10] The K-shell amplitudes at 6.84 MeV predicted in this manner agree with those of Florescu and Gavrila. The L-shell amplitudes predicted using the modified form factor are 15% smaller than those given by the form-factor approximation, confirming the explanation of the discrepancy offered by Kahane, Shahal, and Moreh. Using the modified form factor to predict all the Rayleigh-scattering amplitudes at 6.84 MeV, we obtain a theoretical elastic-scattering cross section of 612 mb/sr in agreement with the experimental value of 633 ± 61 mb/sr.

At photon energies somewhat below 100 keV, in the absence of better predictions, experimental measurements[6,7] have been compared with the form-factor approximation,[16] finding differences especially near the photoeffect K edge. We here report theoretical predictions in agreement with these experiments, which show the breakdown of the form-factor approximation for the K-shell contribution to the scattering. Comparisons of our numerical results with an experiment by Schumacher and Stoffregen[6] for a fixed photon energy of 59.5 keV and atomic numbers 30 through 82 in Fig. 2 shows general agreement at the 5% or better level, in marked contrast to the form-factor predictions which are also shown. In comparisons with an experiment by Tirsell, Slivinsky, and Ebert[7] for scattered photons of energies in the range of 25–75 keV off various heavy atoms, we find somewhat less satisfactory agreement, especially at the scattering angle of 90 degrees, but still a great improvement over the form-factor results. Our predictions for these cases are based on a numerical calculation of the K-, L-, and M-shell Rayleigh-scattering amplitudes and an estimate of higher-shell contributions with the relativistic form-factor approximation. This use of the form-factor approximation is responsible for our indicated theoretical uncertainties, which are especially significant at forward angles.

Our calculations indicate, consistent with the conditions of Bethe's derivation,[17] that the form-factor predictions for the Rayleigh amplitudes will be valid when (1) $(Z\alpha)^2$ is small; (2) the photon energy is greater than about twice the electron's binding energy; and (3) the momentum transfer is small compared to mc. At all energies and angles there are deviations of order $(Z\alpha)^2$, so that form-factor predictions are less accurate in heavy elements. The approximation is not valid for larger angles (high momentum transfers) or lower energies. With decreasing energy the approximation will first fail for inner electrons (of larger binding energy), which, how-

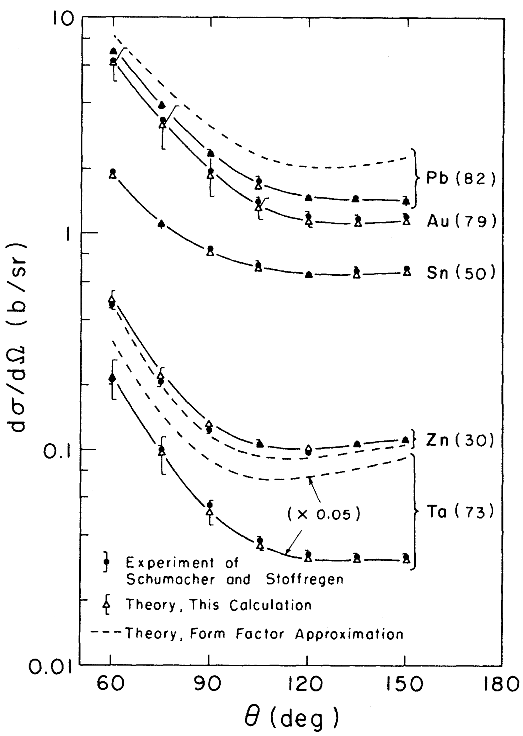

FIG. 2. Differential elastic-photon-scattering cross sections vs scattering angle for 59.5-keV photons scattered by medium to heavy atoms. In addition to their experimental data, the form-factor predictions (dashed lines) quoted by Schumacher and Stoffregen (Ref. 6) are shown for the lightest atom (Zn), the heaviest atom (Pb), and the atom whose K-shell binding energy is closest to 59.5 keV (Ta). The solid line represents cross sections given by our theory.

ever, give a dominant contribution at larger angles. Thus, through the energy regions discussed here, the form-factor approximation may seriously misestimate the angular distributions of an atom, but it will not grossly misestimate the total cross section until L-shell binding energies are reached.

The modified form factor suggested by Brown and Mayers,[10] similar to the form factor for low Z and small momentum transfer, is a superior approximation for the Rayleigh-scattering amplitudes for momentum transfers less than $1mc$. The modified form factor is just as good as the form factor at lower energies and is much more accurate in the high-energy limit. In comparisons of our numerically generated amplitudes with predictions using the modified form factor, we find that even for heavy elements or larger momentum transfers (up to $1mc$) agreement to better than 5% is reached for photon energies greater than about 10–15 times the binding energy for the K shell, with agreement at the 1% level reached by 20 times binding. For higher shells, agreement between numerical amplitudes and those predicted by the modified form factor is at the 1% or better level for photon energies greater than K-shell binding. This excellent agreement at high energies (>10 times K-shell binding) suggests that the modified form factor may be used to predict differential scattering amplitudes for momentum transfers less than $1mc$ for the total atom. At lower energies (1–10 times the K-shell binding), the modified form factor may be used to predict only the contribution made by shells higher than the K shell.

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