Strong correlation effects in atomic photoelectron angular distributions far above thresholds

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We scrutinize individual interchannel coupling effects on atomic dipole and nondipole ($E1$-$E2$) photoelectron angular distribution parameters of valence electrons far above thresholds, choosing $2p$ photoionization of N and Ne in the photon energy range from 1 to 10 keV as case studies. It is found that individual correlation effects are strong far above thresholds. However, a cancellation effect is also discovered that largely obviates the net correlation effect on photoelectron angular distributions. It is shown that the cancellation can be removed, i.e., strong correlation effects can be observed, by considering core-ionized (core-excited) initial states; this is expected to be quite general. The importance of this work is that it shows that the tacit belief in the insignificance of correlation in nondipole parameters far above thresholds is quite misleading. In addition, it suggests studies of core-ionized or core-excited atoms as a means of exploring these large correlation effects in nondipole photoelectron angular distributions far above thresholds.

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I. INTRODUCTION

Recent years have seen an upsurge of activity, both experimental and theoretical, on nondipole effects in photoelectron angular distributions from atoms [1–16], molecules [17], and solids [18,19], which arise from the first-order correction $i\mathbf{k}\cdot\mathbf{r}$ to the dipole approximation for a photoionization matrix element between initial and final states $M_{if} = \langle f|(1+i\mathbf{k}\cdot\mathbf{r})\mathbf{e}\cdot\mathbf{p}|i\rangle$, with $\mathbf{k}$ and $\mathbf{e}$ being the photon momentum and polarization vector, and $\mathbf{r}$ and $\mathbf{p}$ being the electron position vector and the electron momentum operator. The photon energy region under scrutiny has extended from tens of eV to keV energies. The investigations have uncovered various situations where nondipole effects due to electric dipole-quadrupole $E1$-$E2$ interferences, and sometimes even higher-order interferences $E2$-$E2$ and $E1$-$E3$ ($E3$ referring to octupole) are unexpectedly large and *must* be considered to properly account for the photoelectron angular distributions. Remarkably, near threshold, nondipole effects were found to be enhanced largely due to electron-electron correlation [8,9,11]. However, far from thresholds, up to keV photon energies, calculations for rare gas atoms [7,13] found the effects of electron correlation to be unimportant for nondipole effects. This has led to the tacit belief in the general insignificance of electron correlation for nondipole effects far from threshold. As an example, it was recently stated [20] that "In photoeffect angular distributions ... , even when quadrupole effects matter, quadrupole correlations have not been found to be important, except perhaps at threshold ... , which suggests ... a similar situation for Rayleigh scattering."

It is surprising that apparently no consideration has been given to the lack of strong correlation effects in nondipole parameters despite the very strong evidence that correlation in the form of interchannel coupling between an nl subshell ionization amplitude with $l>0$ and amplitudes of inner subshells with $l'<l$ generally must be very important at high energies [21,22]. Indeed, e.g., for the dipole channels, since the single-particle nl cross section falls off as $E^{-l-7/2}$ [23,24], the $n'l'$ cross sections $\sigma_{n'l'}$ with $l'<l$ become more and more dominant compared to σ_{nl}, with increasing energy. Thus the $n'l'$ channels through interchannel coupling, induce greater and greater effects on the nl photoionization channels, with increasing energy. Furthermore, similar considerations apply to the quadrupole channels. As a consequence, e.g., recently [10] strong correlation effects were predicted for β_{3d}, γ_{3d}, and δ_{3d} for Cr at keV photon energies. In view of the above, the weak correlation effects on nondipole parameters in photoelectron angular distributions of a large number of atoms at high energies are puzzling.

It is the purpose of this paper to show that the view that electron correlation contributions to nondipole effects in photoionization (and other processes related to photoionization through the optical theorem) at high photon energies are insignificant is quite misleading. It is demonstrated that correlation effects from individual interchannel couplings on these parameters at high energies are, in fact, very large. However, significant cancellations occur among these large interchannel effects with different channels; this is the reason for the observed insignificance of electron correlation in nondipole parameters at high energies. This is demonstrated by calculations of $2p$ photoionization in N and Ne. It is found that the removal of one (or more) inner shell electron can destroy the cancellation. As a result, the hidden correlation can be observed, so that the net correlation effect in both dipole and $E1$-$E2$ nondipole phototelectron angular distributions becomes extremely strong, even at high energies. To illustrate this, core-ionized atoms are scrutinized. Specifically, we consider $2p$ photoionization of core-ionized N and Ne where the initial states are characterized by an empty or half-empty $1s$ (or $2s$) subshell, and we demonstrate that correlation contributions to dipole as well as to $E1$-$E2$ nondi-

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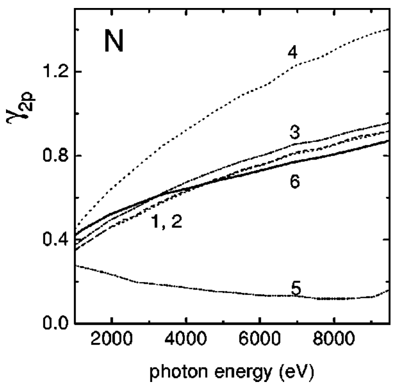

FIG. 1. Nondipole photoelectron angular distribution parameter γ_{2p} for N calculated at different levels of approximation: 1, SPHF; 2, SP RPAE including interchannel coupling between only $2p^3\uparrow$ and $2s\downarrow$ channels (note, that curves 1 and 2 are nearly indistinguishable); 3, SP RPAE including interchannel coupling between only $2p^3\uparrow$ and $1s\downarrow$ channels; 4 SP RPAE including interchannel coupling between only $2p^3\uparrow$ and $2s\uparrow$ channels; 5, SP RPAE including interchannel coupling between only $2p^3\uparrow$ and $1s\uparrow$ channels; 6, full SP RPAE calculation including interchannel coupling among all $1s\uparrow$, $1s\downarrow$, $2s\uparrow$, $2s\downarrow$, and $2p^3\uparrow$ channels.

pole effects in photoionization of these core-ionized atoms in the photon energy region from 1 to 10 keV are extremely strong, in contrast to the effect in neutral ground-state N and Ne atoms.

II. RESULTS AND DISCUSSION

$E1$-$E2$ nondipole effects in photoelectron angular distributions from atoms are conveniently characterized by two asymmetry parameters γ_{nl} and δ_{nl} defined in [2], with δ_{nl} being generally much smaller than γ_{nl} [2,10,13]. It is, therefore, the dominant parameter γ_{nl} that we choose to investigate here as to the importance of correlation in $E1$-$E2$ nondipole effects in core-ionized N and Ne. γ_{nl} depends on interferences between dipole and quadrupole photoionization amplitudes. It is proportional to a linear combination of terms of the form $D_{nl\to\epsilon l'}Q_{nl\to\epsilon l''}\cos(\delta_{l'}-\delta_{l''})$, where the $D_{nl\to\epsilon l'}$'s and $Q_{nl\to\epsilon l''}$'s are the dipole and quadrupole photoionization amplitudes, respectively, with $\delta_{l'}$ and $\delta_{l''}$ being their phases. These amplitudes were calculated, including electron correlation, within the framework of the random phase approximation with exchange (RPAE) [25] for the closed-shell Ne, and the spin-polarized RPAE (SP RPAE) [26,27], for N with a half-filled subshell. Within the SP RPAE, the ground-state configuration of N is characterized as $1s\uparrow 1s\downarrow 2s\uparrow 2s\downarrow 2p^3\uparrow\ {}^4S_{3/2,3/2}$, where arrows indicate electron spin orientations; the spins of all three $3p$ electrons are parallel in the ground state, in accordance with Hund's rule.

In Fig. 1, the results of our calculations for atomic N, at various levels of approximation, are presented. Including no interchannel couplings in calculations of $2p\uparrow$ photoionization amplitudes, i.e., in the framework of the "spin-polarized" Hartree-Fock (SPHF) approximation [28], shown as curve 1, and including interchannel couplings with *all* of the other single excitation channels for both dipole and quadrupole photoionization amplitudes (SP RPAE), shown as curve 6, makes no significant difference between the results for γ_{2p} over a broad energy range, as seen in Fig. 1. This implies that interchannel coupling is quite weak. To understand why the net effect of correlation is weak, in Fig. 1 are shown the calculated results including coupling of photoionization channels of the $2p\uparrow$ subshell with the $2s\uparrow$, $2s\downarrow$, $1s\uparrow$, and $1s\downarrow$ channels individually. Including coupling with either the $2s\uparrow\to\epsilon l\uparrow$ (curve 4) or $1s\uparrow\to\epsilon l\uparrow$ (curve 5) channels has an extremely large effect, as clearly demonstrated in Fig. 1. Note particularly, that coupling with the $2s\uparrow\to\epsilon l\uparrow$ channels dramatically *increases* the value of γ_{2p} from the uncoupled, SPHF, value, while coupling with the $1s\uparrow\to\epsilon l\uparrow$ channels *decreases* γ_{2p} by approximately the same amount. It is, therefore, decidedly incorrect to assume that interchannel coupling is weak; there is, rather, a cancellation between large interchannel effects.

Furthermore, including interchannel coupling of $2p\uparrow\to\epsilon l\uparrow$ with only the spin-down $2s\downarrow\to\epsilon l\downarrow$ (curve 2) or $1s\downarrow\to\epsilon l\downarrow$ channels (curve 3) has a nearly zero effect on γ_{2p}. It is noteworthy, thus, that the interchannel coupling effects are dramatically spin dependent in the sense that the coupling effects on γ_{2p} of the $ns\uparrow$ channels are huge, but the effects of coupling with the $ns\downarrow$ channels are insignificant, i.e., the important interchannel contributions to the nondipole photoionization parameter γ_{2p} for a valence half-filled subshell arise almost exclusively from interaction with channels arising from inner-shell electrons with the same spin orientation as the valence half-filled subshell.

Since the interchannel coupling matrix elements consist of direct and exchange contributions, and exchange contributions vanish for channels with opposite spin orientations, it is evident that the strong interchannel effects must be due to the exchange contributions to the interchannel coupling matrix elements. These exchange contributions clearly dominate over the direct in the high energy region. Indeed, consider the interchannel coupling matrix element between the $2p\uparrow\to\epsilon l\uparrow$ and $2s\uparrow\to\epsilon' l'\uparrow$ channels, i.e., between $1s\uparrow 1s\downarrow 2s\uparrow 2s\downarrow 2p^2\uparrow\epsilon l\uparrow$ and $1s\uparrow 1s\downarrow 2s^0\uparrow 2s\downarrow 2p^3\uparrow\epsilon' l'\uparrow$, which gives

$$\langle 2s\uparrow\epsilon l\uparrow|V|\epsilon' l'\uparrow 2p\uparrow\rangle-\langle 2s\uparrow\epsilon l\uparrow|V|2p\uparrow\epsilon' l'\uparrow\rangle,$$

with V being the interaction Hamiltonian, whereas the interaction of the $2p\uparrow$ ionization channels with $2s\downarrow\to\epsilon' l'\downarrow$, i.e., $1s\uparrow 1s\downarrow 2s\uparrow 2p^3\uparrow\epsilon' l'\downarrow$ gives $\langle 2s\downarrow\epsilon l\uparrow|V|\epsilon' l'\downarrow 2p\uparrow\rangle$ only; the exchange term vanishes. Since the exchange term, in this case, is the one where discrete wavefunctions overlap and continuum wave functions overlap, it is evident that this term will remain much larger, with increasing energy, than the direct term with only discrete-continuum overlap, which decreases rapidly with energy as the continuum wave function becomes more oscillatory. In the exchange term, on the other hand, since the two continuum wave functions have similar energies, they tend to interfere constructively.

These results suggest that core-ionized, or core-excited, N should behave rather differently from ground-state N because, if one of the $ns\uparrow$ electrons is excited or ionized, the

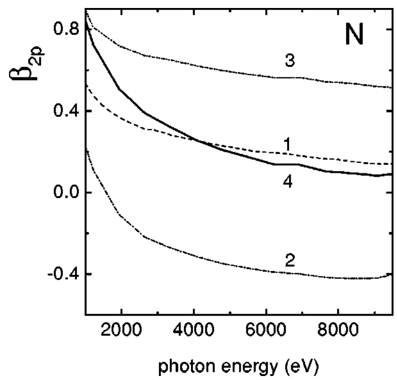

FIG. 2. Dipole photoelectron angular distribution parameter β_{2p} for N calculated at different levels of approximation: 1, SPHF; 2, SP RPAE including interchannel coupling between only $2p^3\uparrow$ and $1s\uparrow$ channels; 3, SP RPAE including interchannel coupling between only $2p^3\uparrow$ and $2s\uparrow$ channels; 4, full SP RPAE calculation including interchannel coupling among all $1s\uparrow$, $1s\downarrow$, $2s\uparrow$, $2s\downarrow$, and $2p^3\uparrow$ channels.

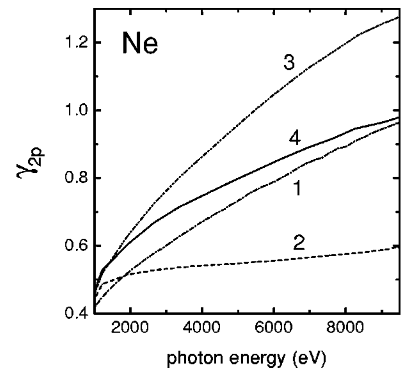

FIG. 3. Nondipole photoelectron angular distribution parameter γ_{2p} for Ne calculated at different levels of approximation: 1, HF; 2, RPAE including interchannel coupling between only $2p^6$ and $1s^2$ channels; 3, RPAE including interchannel coupling between only $2p^6$ and $2s^2$ channels; 4, full RPAE calculation including interchannel coupling among all channels.

cancellation described above can no longer occur; only one of the competitive channels remains. To check on this, calculations of γ_{2p} have been performed on core-ionized N^+,$1s\downarrow 2s\uparrow 2s\downarrow 2p^3\uparrow$ and $1s\uparrow 1s\downarrow 2s\downarrow 2p^3\uparrow$. These results were found to be virtually identical to curves 4 and 5, respectively, in Fig. 1 so they are not shown separately. Nevertheless, these calculations confirm both the previously unsuspected strength of the interchannel coupling correlation effects upon γ_{2p}, and the cancellation that occurs. We note parenthetically that N^+ with a $1s$ hole decays very rapidly ($\sim 10^{-14}$ s) via an Auger process, so it is not a likely experimental candidate. N^+ with a $2s$ hole, on the other hand, is energetically forbidden to decay via an Auger process, and can decay only radiatively with a lifetime of $\sim 10^{-8}$ s [29], which allows for the reasonable possibility that this state could be studied experimentally.

The same considerations should apply to the dipole photoelectron angular-asymmetry parameter β_{nl} [1,2] as well. This is evident from Fig. 2 where calculated results for β_{2p} for atomic N are shown at various levels of calculations, similar to what was shown in Fig. 1 for γ_{2p}. The same strong individual interchannel effects and cancellation are seen as for γ_{2p}. The calculations were also done for coupling with the $1s\downarrow$ and $2s\downarrow$ dipole channels, and, as in the case of γ_{2p}, they produce only insignificant changes in β_{2p}; for the sake of clarity, they are omitted from Fig. 2. Thus, in β as well, individual correlation effects are significant, but they cancel each other out so that the uncoupled and fully coupled results are in substantial agreement. Furthermore, as in the case of γ_{2p}, calculations of $2s\uparrow$ and $1s\uparrow$ core-ionized N^+, i.e., $1s\uparrow 1s\downarrow 2s\downarrow\ p^3\uparrow$ and $1s\downarrow 2s\uparrow 2s\downarrow 2p^3\uparrow$, respectively, gave essentially the same results as curves 3 and 2 of Fig. 2.

To explore if these results are specific to atomic N, or even, more generally, atoms with half-filled subshells, or if the results are of more general applicability, the $2p$ photoionization of the closed-shell Ne($1s^22s^22p^6$) was considered. In Fig. 3, the results of our RPAE and HF calculations for γ_{2p} of Ne from 1 to 10 keV performed at four different levels of approximation are shown. Curve 2 shows γ_{2p} calculated with interchannel coupling only between $1s^2$ and $2p^6$ channels included. It is evident that the influence of $1s^2$ correlation on γ_{2p} is very strong, lowering γ_{2p} compared the uncorrelated HF results (curve 1). Equally strong is the influence of correlation on γ_{2p} when only coupling between $2s^2$ and $2p^6$ channels is included, curve 3; in this case, however, γ_{2p} is strongly increased. In the full RPAE calculation, where interchannel coupling among all excitation channels is taken into account, curve 4, the net effect of correlation on γ_{2p} decreases markedly. Thus, as in the case of atomic N, γ_{2p} of Ne exhibits strong cancellation between the modification of the $2p$ transition matrix elements owing to interchannel interactions with the $2s$ photoionization channel, on one hand, and interactions with the $1s$ channel, on the other.

Also, as in the case of N, we have investigated $2p$ photoionization of core-ionized Ne^+, working in both $1s^22s2p^6\ ^2S$ and $1s2s^22p^6\ ^2S$ states. Since we are dealing with a half-filled s subshell, in each case it was necessary that the spin-polarized formulation be used, as was applied to N. For each initial state we investigated both $2p\downarrow$ and $2p\uparrow$ photoionization, which, assuming $ns\uparrow$ for unpaired electron in the initial states, leads to ^3P and ^1P states of Ne^{2+}, respectively. The results followed exactly what was found in the case of N. For the ^1P final states ($2p\uparrow\rightarrow\epsilon l\uparrow$), the exchange term remained and the results were virtually the same as for neutral Ne, including the cancellation. For the ^3P final states ($2p\downarrow\rightarrow\epsilon l\downarrow$), the exchange term with the unpaired ns electron vanished, and the cancellation vanished as well, leading to results almost exactly like those in the neutral Ne case with coupling between $2p$ and $2s$ channels omitted. Again, as in the case of N, since the results are so close those for to neutral Ne, they are not shown.

To understand the origin of the approximate cancellation of interchannel coupling effects on $2p$ ionization by $2s$ and $1s$ channels, note that the major correction, to a $2p\rightarrow\epsilon l$ transition matrix element $\langle 2p|T|\epsilon l\rangle$ induced by interchannel coupling with a $ns\rightarrow\epsilon' l'$ channel is proportional [21,22,24] to $\langle 2p(1)\epsilon' l'(2)|V|ns(1)\epsilon l(2)\rangle\langle ns|T|\epsilon' l'\rangle$ with ϵ' taking on the value implied by energy conservation. The transition matrix element $\langle 1s|T|\epsilon' l'\rangle$ is much larger than $\langle 2s|T|\epsilon' l'\rangle$ for keV photon energies, and both are positive [23]. On the other hand, the interchannel coupling matrix element $\langle 2p(1)\epsilon' l'(2)|V|2s(1)\epsilon l(2)\rangle$ is much larger than $\langle 2p(1)\epsilon' l'(2)|V|1s(1)\epsilon l(2)\rangle$. This is because the $2p$ and $2s$ wavefunctions overlap much better than $2p$ and $1s$, and for the $2s$ case ϵ' and ϵ are approximately the same, leading to constructive interference between the continuum wave functions. In addition, the $2p$ overlap with $2s$ is negative, while the overlap with $1s$ is positive. This means that the interchannel coupling matrix element with the $2s$ channel is much larger in magnitude than, and of the opposite sign to, the interaction with the $1s$ channel. The products of the interaction and transition matrix elements, the correction to the $\langle 2s|T|\epsilon l\rangle$ amplitude, are, thus, about the same magnitude and of opposite sign, leading to the approximate cancellation found.

III. CONCLUSION

We have shown that electron correlation contributions in the form of interchannel coupling to photoelectron angular distribution parameters for $2p$ photoionization from N and Ne at photon energies far above threshold are quite strong but exhibit dramatic cancellation effects. Certain core-ionized states also exhibit this cancellation, while in others the cancellation does not exist. This was traced to the dominant part of the interchannel coupling matrix element between $2p$ and ns ionization channels, the exchange term, which vanishes when the spins of $2p\rightarrow\epsilon l$ and $ns\rightarrow\epsilon' l'$ channels are opposite. It was suggested that the $2s$ core-ionized state of N exists long enough to be amenable to experimental investigation. It is also evident, based on the explanation of the phenomenon, that *core-excited* states will exhibit the same sort of behavior as core-ionized states.

The cancellation was explained in terms of the dominant corrections to the uncorrelated transition amplitude induced by interchannel coupling. From this explanation, it seems likely that the cancellation phenomenon can be removed and thus correlation effects on photoelectron angular distribution parameters will be observable for all the elements from B to Ne. In addition, it is probable that the phenomenon will extend to higher-Z elements as well. Moreover, since the limitations of the cancellation effect remain largely unknown, calculations of nondipole effects at energies far above thresholds that omit correlation must be carefully scrutinized to ascertain their accuracy. We are currently extending our studies to higher-Z elements.

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