Principal-quantum-number dependence of coherence and correlation parameters for excitation of helium by electrons

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Electron-photon coherence and correlation parameters for electron-impact excitation of the $n\,^1P$ ($n=2$–8) states of helium at 80 eV are predicted to be essentially independent of the principal quantum number (n), and the available experimental data for $n=2$ and 3 show (semiquantitatively) the same behavior. The n independence of these parameters predicted by first-order many-body theory can be explained using basic concepts associated with quantum-defect theory and, if verified by further experimental results, has important consequences for understanding the physics of the electron-atom scattering process.

A number of experiments involving electron-photon coincidence with atomic targets have been reported since the pioneering work of Eminyan *et al.*[1,2] The vast majority of these experiments have examined the electron impact excitation of the $2\,^1P$ or $3\,^1P$ states of helium although results involving neon, argon, krypton, mercury, sodium, and hydrogen have been reported recently.[3,4] The first set of coherence and correlation parameters, denoted by λ and χ, were introduced by Eminyan *et al.*[1,2] to treat excitation of the $n\,^1P$ ($n=2,3,\ldots$) states of helium. They defined λ and χ by

$$\lambda=\frac{|a_0|^2}{|a_0|^2+2|a_1|^2},\quad a_M=|a_M|e^{i\chi_M},\quad \chi=\chi_1-\chi_0 \qquad (M=0,\pm1) \qquad (1)$$

where a_M denotes the scattering amplitude for the excitation of the Mth ($M=0,\pm1$) sublevel of the $n\,^1P$ electronic state. Calculations of the λ and χ parameters have been reported using distorted-wave theories, first-order many-body theory (FOMBT), distorted-wave polarized-orbital approximations, multichannel eikonal theory, and the R-matrix method.[5,6] Because of simpler physical interpretations[7,8] emphasis has recently been placed on using the equivalent $\langle L_\perp\rangle$ and γ parameters, which are defined by[7,8]

$$\langle L_\perp\rangle=-2[\lambda(1-\lambda)]^{1/2}\sin\chi\ ,$$
$$\tan(2\gamma)=-2[\lambda(1-\lambda)]^{1/2}\cos\chi/(2\lambda-1)\ . \qquad (2)$$

The purpose of this paper is to report that the coherence and correlation parameters for excitation of the $n\,^1P$ ($n=2$–8) electronic states of helium, at an incident electron energy of about 80 eV, are predicted to be essentially independent of the principal quantum number (n) for all scattering angles. These new predictions for the $\langle L_\perp\rangle$ and γ parameters were obtained using the FOMBT (Ref. 9) with the slight modification that the transition density matrix was calculated using "fixed-core" Hartree-Fock (HF) wave functions[10] for the atomic target states.

Figures 1 and 2 compare the theoretical results for the $\langle L_\perp\rangle$ and γ parameters (respectively) for excitation of the $n\,^1P$ ($n=2$–8) states of helium with the available experimental data for excitation of the $2\,^1P$ and $3\,^1P$ states and with the R-matrix calculation results of Fon *et al.*[11] in the $2\,^1P$ case. From these figures it is clear that the coherence and correlation parameters calculated by FOMBT are essentially independent of the principal quantum number (n). We note that the experimental data for $n=2$ and 3 in Figs. 1 and 2 also suggest an n independence although the error bars are currently too large to be certain. We note that if the $\langle L_\perp\rangle$ and γ parameters are n independent, then so will be the λ and χ parameters, and vice versa.

This predicted n independence can be understood by examining both the direct and exchange scattering T matrices. The "direct" portion of the FOMBT T matrix (T^D) for excitation of the $n\,^1P$ states of helium can be written in terms of the radial integrals,

$$T^D_{kl',k'l'}=\int_0^\infty P_{kl}(r)P_{k'l'}(r)V_{1s\to np}(r)dr\ , \qquad (3)$$

where $P_{kl}(r)$ is a continuum Hartree-Fock (static-exchange) orbital with energy k^2 (in Ry) and angular-momentum quantum number l, and $V_{1s\to np}(r)$ is defined by

$$V_{1s\to np}(r)=\frac{1}{r^2}\int_0^r P_{1s}(r')P_{np}(r')r'dr' + r\int_r^\infty P_{1s}(r')P_{np}(r')\frac{dr'}{r'^2}\ , \qquad (4)$$

where $P_{1s}(r)$ is the ground-state HF orbital and $P_{np}(r)$ is the fixed-core HF orbital of the $n\,^1P$ electronic state. The cause of the weak n dependence of the $\langle L_\perp\rangle$ and γ parameters can be traced to the weak n dependence of both $V_{1s\to np}(r)$ and $P_{k'l'}(r)$. It is to be noted that only the behavior of the $P_{np}(r)$ orbital where $P_{1s}(r)$ is nonzero is important in Eq. (4) and in this small-r region the only strong n dependence in $P_{np}(r)$ comes through the orbital normalization constant.[22] According to quantum-defect theory (QDT), one can write $P_{np}(r)$ in the form[23]

$$P_{np}(r)=(-1)^n\left[\frac{\nu_n^3(1+C_n)}{2}\right]^{-1/2}P(E_n,r)\ , \qquad (5)$$

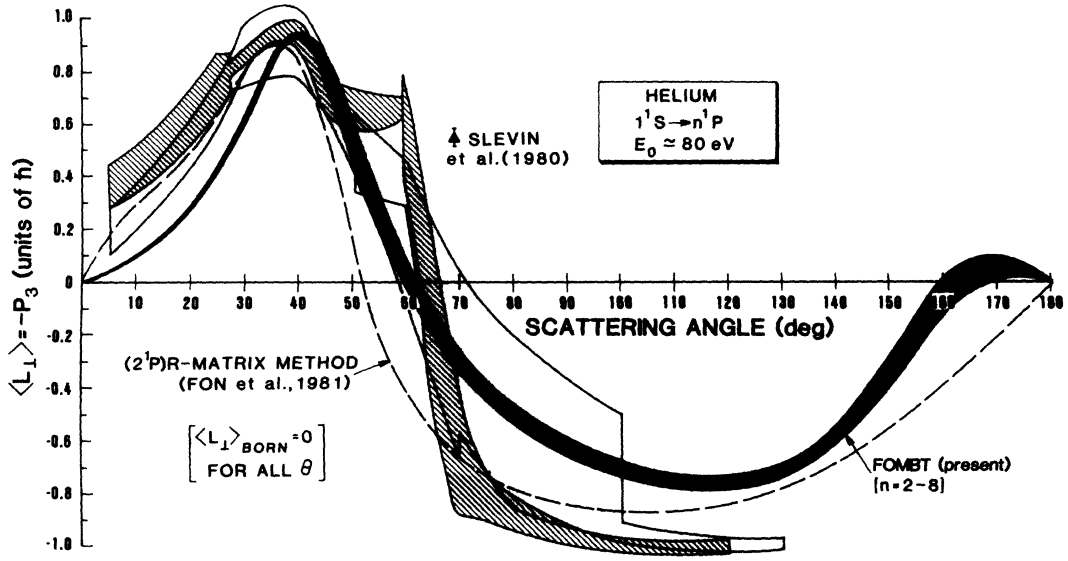

FIG. 1. The $\langle L_\perp \rangle$ parameter, as a function of the scattering angle, for excitation of the $n\,^1P$ states of helium by 80 eV energy electrons. The darkest shaded region denotes the present FOMBT results ($n=2$–8); the lightly speckled regions denote the experimental data for the $2\,^1P$ state (Refs. 1, 2, 12–14, and 19–21); the cross-hatched regions denote the data for the $3\,^1P$ state (Refs. 15–19).

where the effective quantum number ν_n is defined by $\nu_n = n - \mu_n$. μ_n is the quantum defect, and the energy of the $n\,^1P$ state E_n is given by[23]

$$E_n = \frac{-me^4}{2\hbar^2}\frac{Z^2}{(n-\mu_n)^2} = \frac{-me^4}{2\hbar^2}\frac{Z^2}{\nu_n^2} \quad (Z=2 \text{ for helium}), \tag{6}$$

and C_n is defined as[23] $C_n = C(\nu_n)$ with $C(\nu) = d\mu/d\nu$.

The function $P(E,r)$ is an analytic function of E in the small-r region. Thus we can write

$$P(E_n,r) = P(0,r) + E_n \left.\frac{dP(E,r)}{dE}\right|_{E=0} + \cdots . \tag{7}$$

In the *lowest-order* approximation, the energy dependence of both the qauntum defect and $P(E_n,r)$ can be neglected to yield

$$V_{1s\to np}(r) = \left[\frac{\nu_n^3}{2}\right]^{-1/2}(-1)^n \left[\frac{1}{r^2}\int_0^r P_{1s}(r')P(0,r')r'dr' + r\int_r^\infty P_{1s}(r')P(0,r')\frac{dr'}{r'^2}\right]$$
$$\equiv \left[\frac{\nu_n^3}{2}\right]^{-1/2}(-1)^n V_{1s,p}(r) , \tag{8}$$

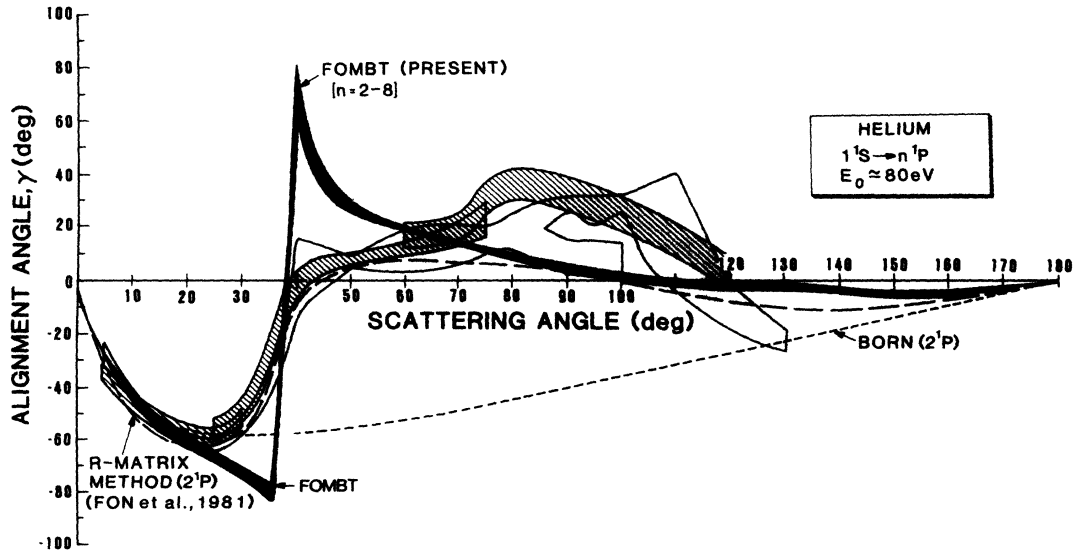

FIG. 2. The γ parameter, as a function of scattering angle, for excitation of $n\,^1P$ states of helium by 80 eV energy electrons. The notation used for the other two shaded regions is the same as used in Fig. 1. The apparent "cusps" in the FOMBT results near $\theta = 40°$ are an artifact of the phase convention choosen for determining γ from Eq. (2).

and thus

$$T^D_{kl,k'l'} = \left[\frac{\nu_n^3}{2}\right]^{-1/2} (-1)^n T^{D,\mathrm{red}}_{kl,k'l'} , \tag{9}$$

where $T^{D,\mathrm{red}}_{kl,k'l'}$ depends on n only through k'.

The above result shows that, in the lowest-order approximation, the ratio $V_{1s\to np}(r)/V_{1s\to n'p}(r)$ is a contant. In a numerical study using the complete expression, we found that for $n=2$ and $n'=6$ this ratio changes by less than 20% from $r=0$ to 6 a.u. and by less than 1% from $r=6$ to 30 a.u. For r values that are larger than the extension of the atomic $1s$ orbital (i.e., for $r>6$ a.u.), it can be shown that this ratio is constant for the accurate $V_{1s\to np}(r)$ potential and, in calculating $T^D_{kl,k'l'}$ for low l partial waves ($l,l'=0,1,2,3$), the influence of the larger-r values of $V_{1s\to np}(r)$ is most important for the accurate parameterization of the T matrix. For small-r values in $V_{1s\to np}(r)$, the (weak) E_n dependence becomes relatively more important and has an influence for large scattering angles.

An additional n dependence enters $T^D_{kl,k'l'}$ via the $P_{k'l'}(r)$ orbital through the energy of the scattered electron $k'^2=k^2-(E_n-E_{1^1S})$. It can be shown that $T^D_{kl,k'l'}$ depends only on the ratio k'/k if spherical Bessel functions are used for $P_{k'l'}(r)$ and the asymptotic form for $V_{1s\to np}(r)$. In the intermediate-energy region, the energy of the $2\,^1P$ state differs by about 5% from the ionization potential, and therefore, the k'/k ratio will introduce only a weak n dependence.

We note here that both the Born and Glauber approximations[2] give $\lambda=\cos^2\theta_K$ and $\chi=0$ (and also $\gamma=-\theta_K$) where θ_K is the polar angle of the transferred momentum $\mathbf{K}=\mathbf{k}'-\mathbf{k}$ relative to the incident momentum, $\mathbf{k}$. As a consequence, coherence and correlation parameters obtained with these scattering models are *exactly* n independent if λ and χ are plotted as functions of θ_K and not the scattering angle θ. This indicates that in general, one might obtain a more pronounced n independence for λ and χ if they were plotted as functions of θ_K.

The exchange T-matrix element (T^E) can be analyzed in a similar fashion and, since T^E contributes relatively little to the total T matrix, the energy dependence of the scattered electron orbital can be completely neglected. If Eqs. (5) and (7) are used, we obtain in the *lowest-order* approximation

$$T^E_{kl,k'l'} = \left[\frac{\nu_n^3}{2}\right]^{-1/2} (-1)^n T^{E,\mathrm{red}}_{kl,k'l,} , \tag{10}$$

where $T^{E,\mathrm{red}}_{kl,k'l'}$ depends on n only through k'. Thus in zeroth-order approximation, we obtain the same n dependence for $T^D_{kl,k'l'}$ and $T^E_{kl,k'l'}$. Therefore, Eqs. (9) and (10) show that the λ and χ parameters will be approximately independent of n because these parameters involve *ratios* of the magnetic sublevel T matrices and the multiplying factor $(\nu_n^3/2)^{-1/2}(-1)^n$ cancels from the ratio. For the exact T matrices, however, a weak n dependence will enter λ and χ through the n dependence of $P(E_n,r)$ and $P_{k'l'}(r)$ functions. One may extend this analysis to second-order many-body theory (SOMBT) (Refs. 24 and 25) and show, that in the adiabatic limit, the second-order transition potential essentially reduces to a form given by Eq. (4) except that $P_{1s}(r)$ is replaced by a "polarized" $1s$ orbital for which the spatial extent does not differ signficiantly from that of the $1s$ orbital. Therefore, the argument used following Eq. (4) is also valid in this case and indicates that SOMBT, at least in the adiabatic limit, will also demonstrate the n independence predicted by FOMBT. It is more difficult to make predictions about conventional distorted-wave (DW) theory[26,27] or that version of it[27] which uses distortion potentials of the final (excited) state for both incident and scattered electrons. In these theories, the incident and scattered electron orbitals also depend on n through the distortion potential, but this is expected (in most cases) to introduce only a weak n dependence. However, close to resonances and to the excitation threshold, the effect of the excited state potential can be significant and therefore may cause a stronger n dependence in the associated T matrix beyond the one in the normalization constant.

The n independence of the correlation and coherence parameters predicted by the FOMBT may have a broader significance than these results alone. We noted above that the *experimental results* shown in Figs. 1 and 2 do indeed appear to be approximately independent of n. If the predicted n independence (for an incident electron energy above threshold and away from the resonance regions) is indeed verified by more extensive experimental measurements, it establishes the following.

(i) The strong n dependence for the exact T matrix can be factored out so that ratios of the various magnetic sublevel T matrices are indeed independent of the principal quantum number (n).

(ii) Integral cross sections for excitation of *any* n can be calculated, for incident electron energies above threshold and away from resonances, by using this n scaling (approximately ν_n^{-3}) and the best available experimental or theoretical data for $n\lesssim 3$. It is important to note that this is not just a high-energy or large-n scaling relationship but is limited only by the accuracy of the scattering model or the experimental data being extrapolated to larger n values.

(iii) The electron-photon coincidence characteristics for an excited state of a particular symmetry can be measured accurately by choosing a specific (and perhaps different) n value for which the associated optical emissions can be easily measured (e.g., the visible), rather than be restricted to emissions from the specific state of interest.

We note here that the dependence of $\langle L_\perp \rangle$ on the scattering angle predicted by FOMBT agrees better with experiment than does the predicted γ dependence. The fact that no theoretical model correctly predicts the measured increase in γ for scattering angles $40°\lesssim\theta\lesssim 110°$, indicates that the observed increase in γ is apparently due to some physical interaction yet to be identified although the data in Figs. 1 and 2 appear to approximately satisfy the predicted n independence.

Additional measurements (as well as calculations with more elaborate theories) of the coherence and correlation parameters in helium (for $n\gtrsim 3$) and other atomic targets are needed to test the predictions made in this paper.

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