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# POSITRON EXCITATION OF NEON

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## ABSTRACT

The differential and total cross section for the excitation of the 3s $^1P_1^o$ and 3p $^1P_1$ states of neon by positron impact have been calculated using a distorted-wave approximation. Our results agree well with experiment.

## THEORY

We are continuing our earlier work on the positron excitation of the noble gases[1,2] by calculating cross sections for the excitation of the 2p$^5$ ($^2P^o_{1/2}$) 3s $^1P_1^o$ as well as the 2p$^5$ ($^2P^o_{1/2}$) 3p $^1P_1$ states of neon. We use a distorted wave approximation similar to our former calculations on helium.

In the incident channel the distortion potential consists of the static potential plus the polarized-orbital polarization potential used previously for elastic scattering.[3] In the excited channel the distortion potential consists of the appropriate static potential plus a polarization potential determined by an extension of Stone's method.[4]

In order to calculate this potential we construct the following polarized orbital:

$$\psi_{nlm}(\boldsymbol{r},\boldsymbol{x}) = \varphi_{nlm}(\boldsymbol{r}) + \sum_{\substack{n'l'm' \\ \lambda'\mu'}} \varphi_{n'l'm'}(\boldsymbol{r})\,\beta^{n'l'}_{\lambda'}(x)\,Y_{\lambda'\mu'}(\hat{\boldsymbol{x}})\,(l'm'\lambda'\mu' \mid l'\lambda' lm) \tag{1}$$

where the $\varphi_{nlm}(\boldsymbol{r})$ are the unperturbed states of the atom and $\boldsymbol{r}$ represents the coordinates of all the bound electrons. The positron coordinate is represented by $\boldsymbol{x}$ and the symbol $(l'm'\lambda'\mu' \mid l'\lambda' lm)$ is the usual vector-coupling coefficient.

We define the adiabatic hamiltonian $H_{\text{ad}}$ as

$$H_{\text{ad}} = H_{\text{atom}} + V(\boldsymbol{r},\boldsymbol{x}) \tag{2}$$

where $H_{\text{atom}}$ is the hamiltonian of the unperturbed atom and $V(\boldsymbol{r},\boldsymbol{x})$ represents the perturbation due to the incident positron. The unknown coefficients $\beta^{nl}_{\lambda}$ are then determined from the set of equations

$$\langle \varphi_{nlm}(\boldsymbol{r}) \mid H_{\text{ad}} - E(\boldsymbol{x}) \mid \psi_{nlm}(\boldsymbol{r},\boldsymbol{x})\rangle = 0 \tag{3a}$$

and

$$\Big\langle \sum_{m''\mu''} \varphi_{n''l''m''}(\boldsymbol{r})\,Y_{\lambda''\mu''}(\boldsymbol{x})\,(l''m''\lambda''\mu'' \mid l''\lambda'' lm) \mid H_{\text{ad}} - E(\boldsymbol{x}) \mid \psi_{nlm}(\boldsymbol{r},\boldsymbol{x})\Big\rangle = 0 \tag{3b}$$

for all values of $n''l''$ and $\lambda''$ in the sum in (1). The angle brackets indicate integration over the electron coordinates only. The set of equations (3) are expanded in spherical harmonics and the various terms in the perturbed energy $E(\boldsymbol{x})$ are eliminated. Sufficient numbers of the lowest order equations from the set (3) are retained in order to solve for the unknown functions $\beta^{nl}_{\lambda}$. Note that these are *algebraic* equations for the unknown functions.

In the present work we restrict the sum in equation (1) to a single term by taking $\lambda' = 1$ and $\varphi_{n'l'm'}$ as the 3s $^1P_1^o$ state when $\varphi_{nlm}$ represents the 3p $^1P_1$ state and vice versa. We note that the 2p$^5$3p configuration gives rise to 3 possible multiplets, viz $^1D$, $^1P$ and $^1S$ so that other choices for the polarized orbital are possible. With our particular choice the polarization potential becomes

$$V_{\text{p}}(x) = -\frac{1}{4\sqrt{\pi}}\,\beta(x)\,\frac{1}{x}\,y_1(3\text{s},3\text{p};x) \tag{4}$$

for both states although the value for $\beta$ differs in the two cases.

The distorted-wave $T$-matrix for the excitation is then given by

$$T(nlm \to n'l'm') = \langle \varphi_{n'l'm'}(\boldsymbol{r})\,\chi_f^-(\boldsymbol{x}) \mid V(\boldsymbol{r},\boldsymbol{x}) \mid \varphi_{nlm}(\boldsymbol{r})\,\chi_i^+(\boldsymbol{x})\rangle \tag{5}$$

where $\chi_i^+$ and $\chi_f^-$ are the distorted-waves in the incident and final channels respectively.

In the case of excitation to the 3p $^1P_1$ state the cross section for the $m = 0$ magnetic sublevel is zero. This means that the differential cross section for this transition is zero for a scattering angle of 0° or 180°. The cross section also displays a dip near 90° at most energies. We show some typical results in figure 1.

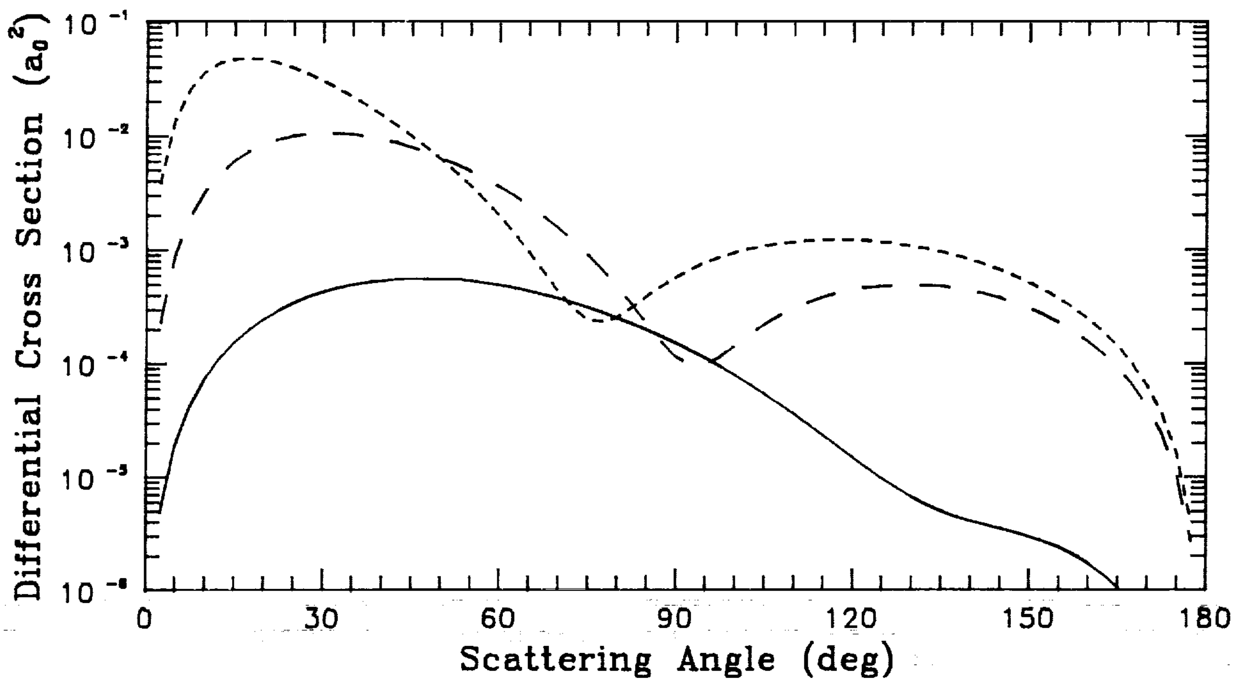


FIG. 1. Differential cross sections for the excitation of the 3p $^1P_1$ state of neon by positron impact at 20 eV, (——); 25 eV, (– – –); and 40 eV, (- - -).

For the excitation of the 3s $^1P_1^o$ state the differential cross sections decrease monotonically with angle.

The integrated cross sections for these two transitions are shown in figure 2 along with the experimental data.[5] The theoretical values for the excitation of the 3s $^1P_1^o$ state are comparable in magnitude to the experiment results. The cross sections for the 3p $^1P_1$ state are about a sixth of the magnitude of the ones for the 3s $^1P_1^o$ state.

In comparing the theoretical and experimental results the following points should be noted. The experiment was based upon a time-of-flight technique which only measured scattering in the forward direction (approximately up to 60°). However, since the differential cross sections are peaked in the forward direction this does not introduce an appreciable error. It also measured all the positrons which arrived at the detector within the specified time period. Thus positrons exciting a variety of states were included and the measured cross section is a sum of these.

On the theoretical side, the cross sections for the excitation of the 3p $^1D_1$ and 3p $^1S_1$ states should also be taken into account when comparing with experiment. These latter cross sections are expected to be of the same order of magnitude as for the 3p $^1P_1$ state. Excitation to higher states are not very important as the higher threshold energies for these states means a longer time-of-flight and hence a smaller proportion of the cross section was measured.

In conclusion, while the overall magnitude of our calculated cross sections agree quite well with the experimental data more detailed measurements will be necessary before more quantitative conclusions can be made.

## ACKNOWLEDGMENTS

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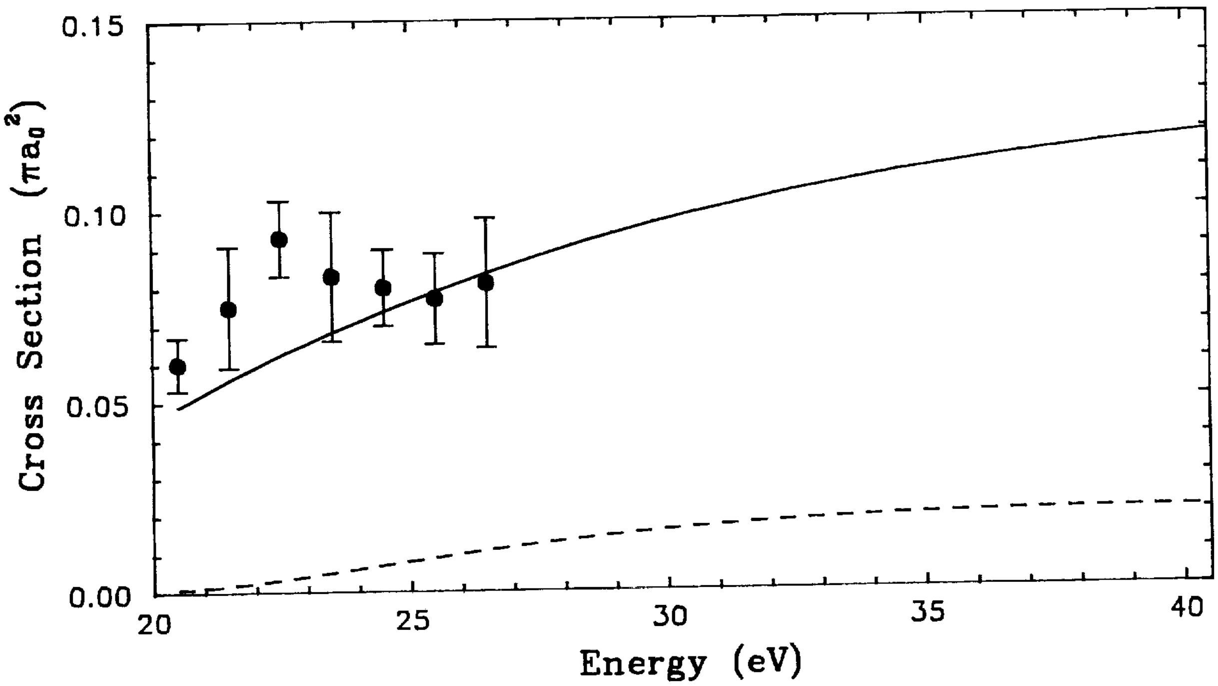


FIG. 2. Integrated cross sections for the excitation of neon by positron impact: (——), excitation of the 3s $^1P_1^o$ state; (– – –), excitation of the 3p $^1P_1$ state; (•), experiment.[5]

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