

Calculations of electron shakeoff probabilities using pseudostates

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Synopsis Electron shakeoff probabilities accompanying inner-shell vacancy production are calculated in the screened hydrogenic model using pseudostates. The results are compared with the values calculated with continuum wave functions.

When an inner-shell vacancy is created, other electrons in the same atom experience sudden change in the central potential and have a probability to be ejected from the atom. This process is called *shakeoff* and has been extensively studied both theoretically and experimentally.

In the sudden approximation, the shakeoff probability can be given in terms of imperfect overlap between the initial- and final-state wave functions. However, the final state corresponds to the continuum state and calculations involving continuum wave functions are sometimes complicated and tedious. It is interesting to calculate electron shakeoff probabilities with a simpler approach.

In the present work, we use the pseudostate method and calculate the shakeoff probability in the screened hydrogenic model. For this model, the shakeoff probabilities with continuum wave functions are known in the simple analytical forms [1]. We consider a Schrödinger equation for hydrogenic potential and expand the eigenfunction $\varphi(r)$ in terms of a set of basis functions:

$$\varphi(r) = \sum_{i=1}^N c_i \chi_i(r),$$

where N is the number of basis set, c_i is the expansion coefficient and $\chi_i(r)$ is the Slater-type orbital (STO). With suitable choice of N and parameters of STO's, the atomic Hamiltonian is diagonalized and the energy eigenvalues of the hydrogenic atom are well reproduced. In addition to these bound states, we obtain states with positive discrete energy, i.e. *pseudostates*. The eigenfunctions corresponding to pseudostates in the final state are used to calculate the overlap integral with the initial bound-state wave function. The basis set consists of ten STO's both for $l = 0$ and $l = 1$. The screening constants are obtained according to the Slater's recipe.

Figure 1 shows the comparison of the pseudostate wave function of Ne for the energy eigenvalue $E = 4.83$ a.u. and $l = 0$ with the corresponding continuum wave function. The former is normalized to the latter at the first peak. It is clear that both wave functions have similar shape.

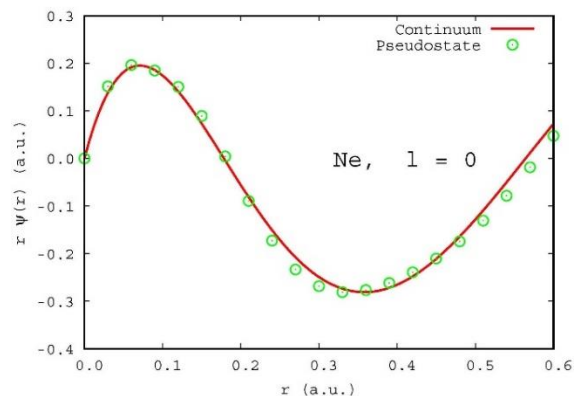


Figure 1. Comparison of the pseudostate wave function of Ne for $E = 4.83$ a.u. and $l = 0$ with the corresponding continuum wave function.

The shakeoff probability is calculated as the sum of overlap integrals for the pseudostates. The results for Ne accompanying K-shell vacancy production is shown in Table 1 and compared with the values obtained with continuum wave functions [1].

Table 1. Electron shakeoff probabilities for Ne accompanying K-shell vacancy production (%).

	1s	2s	2p
Pseudostate	0.028	1.18	1.35
Continuum	0.029	1.12	1.41

The present results indicate that the pseudostate approach is useful to calculate the electron shakeoff probabilities accompanying inner-shell vacancy production.

References

[1] T. Mukoyama, 2005 *X-Ray Spectrom.* **34**, 64.

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