

A NOTE ON: LOW ENERGY SCATTERING OF ELECTRONS BY
POTASSIUM ATOMS

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ABSTRACT

The R-matrix method is applied to calculate eigenphase sums and total cross sections for electrons incident on potassium atoms with energies from 0 - 3.5 eV. The three state (4s-4p-3d) all electrons calculation is used to describe the scattering process.

INTRODUCTION

The study of low energy scattering of electrons by alkali-metal atoms has received much attention, both theoretically and experimentally, over the last thirty years. The atomic beam recoil technique has been used [1] to measure total cross sections for the scattering of electrons by lithium, sodium and potassium. Using the same technique visconti et al [2] measured the absolute total cross section for the scattering of electrons in the energy range 0.3-9 eV by potassium, rubidium and cesium. Slevin et al [3] employed a new method for obtaining absolute differential excitation cross sections in low energy electron atom scattering. Their new method utilizes certain of the kinematic properties of a recoiling-atom beam in an electron-

Delta J. Sci. 15 (3) 1991

Low Energy Scattering

atom crossed-beam configuration to distinguish between elastic scattering and excitation to various atomic levels. They applied the new method to study the electron-potassium scattering at 3,4.4 and 5.2 eV.

The two state (4s-4p) close coupling approximation is used [4] for studying elastic scattering of electrons by alkali-metal atoms. The variational form of solution of continuum Bethe-Goldstone equations is employed [5] to compute elastic total and exchange cross sections for electron scattering by Li, Na and K at energies below the first excitation threshold. In the frozen core Glauber approximation, Walters [6] calculated cross sections for elastic scattering and excitation of the resonance transitions in Li, Na and K. A three state (4s-4p-3d) close coupling approximation is applied [7] to the scattering of electrons with energies of up to 5 eV by potassium atoms. The Vainshtein approximation with exchange via the Ochkur-Rudge method and Ochkur's modified first Born approximation are used [8] to calculate excitation cross sections of Li, Na and K. Position and width of the resonance in electron-potassium scattering from self broadening of Rydberg states are obtained [9].

In the present calculations was use the three state R-matrix method to calculate phase shifts and total elastic and excitation cross sections in electron-potassium scattering.

THEORY

The analytic form of the linear combination of Slater type orbitals

$$P_{nl}(r) = \sum_{i=1}^k C_{inl} r^{I_{inl}} \exp(-\xi_{inl} r) \quad (1)$$

is used to express the radial part of the core and valence wave functions of the atomic electrons, where C_{inl} and I_{inl} are linear coefficients and ξ_{inl} is a nonlinear exponent. P_{nl} is determined using the general atomic structure code of Hibbert [10]. In this calculation we included the three target states (1s 2s 2p 3s 3p 4s) $2S^e$, (1s 2s 2p 3s 3p 4p) $2P^o$ and (1s 2s 2p 3s 3p 3j) $2D^e$. The (N + 1)- total electron wave function is written in the form

$$\Psi_R = A \sum_{ij} c_{ijk} \Phi_i V_j + \sum_j d_{ik} \Phi_j \quad (2)$$

where Φ_i are a finite set of atomic eigenstates which diagonalize the atomic Hamiltonian, these atomic eigenstates are combined here with the angular and spin function for the incident electron to form channel eigenstates of L^2 and S^2 and their Z -components. The finite set of continuum orbitals, V_j , corresponding to the appropriate orbitals angular momentum, describing the motion of the scattered electron, are obtained by solving the equation (for details see reference 11) :

Delta J. Sci.15 (3) 1991

Low Energy Scattering

$$\left(\frac{d^2}{dr^2} - \ell(\ell+1) / r^2 + V(r) + k_i^2 \right) v_i(r) = \sum_j \lambda_{ij} P_j(r) \quad (3)$$

with

$$V(r) = 2Z/r \exp(-Z^{1/3}, r), \quad (4)$$

$Z = 19$ in case of potassium.

The λ_{ij} are Lagrange undetermined multipliers. Turning again to equation (2), the ϕ_j are (N+1)-electron configurations formed from the atomic orbital basis. Finally the coefficients c_{ijk} and d_{ik} are determined by diagonalizing the (N+1)-electron Hamiltonian.

Equation (3) is solved subject to the R-matrix boundary conditions:

$$v_i(0) = 0$$

$$v'_i(a) / v_i(a) = b/a$$

and the orthonormality condition

$$\int_0^a v_i(r) v_j(r) dr = \delta_{ij}$$

The continuum orbitals were determined by imposing a logarithmic derivative of zero at the R-matrix radius $a=30.16$ au and these continuum orbitals are lagrange orthogonalized to the 1s, 2s, 2p, 3s, 3p, 4p, 3d Hartree-Fock orbitals. In the energy range of interest adequate convergence was obtained by retaining eighteen continuum orbitals for each angular momentum.

Delta J. Sci. 15 (3) 1991

O. Nagi

RESULTS AND DISCUSSIONS

We give in figure (1) the results of calculation of the eigenphase sums. Eigenphases of S- and P-waves, obtained by diagonalizing the S-matrix, are in close agreement with Karule [4] below the 4p threshold. For D-wave there is a small difference due to our inclusion of the 3d-state into the calculation. The S-wave eigenphase sums rise very rapidly to threshold. The i_p^o eigenphase sum has a sharp resonance just below the excitation threshold due to the 4s 4p i_p^o configuration. Also there is a resonance located close to 4s threshold caused by the 4s 4p 3P_o configuration. Turning to the D-waves we find two resonant states close to 4p and 3d thresholds in the iD^e eigenphase sum. These resonances are due to 4P_e iD^e and 3d^e iD^e configurations, respectively.

In figures (2) and (3) , we show the total cross sections for 4s \rightarrow 4s and 4s \rightarrow 4p transitions compared with Moores results [7]. A few sharp features appear in our total cross sections because of resonances identified from the eigenphase sums. Our results are in good agreement with Moores [7].

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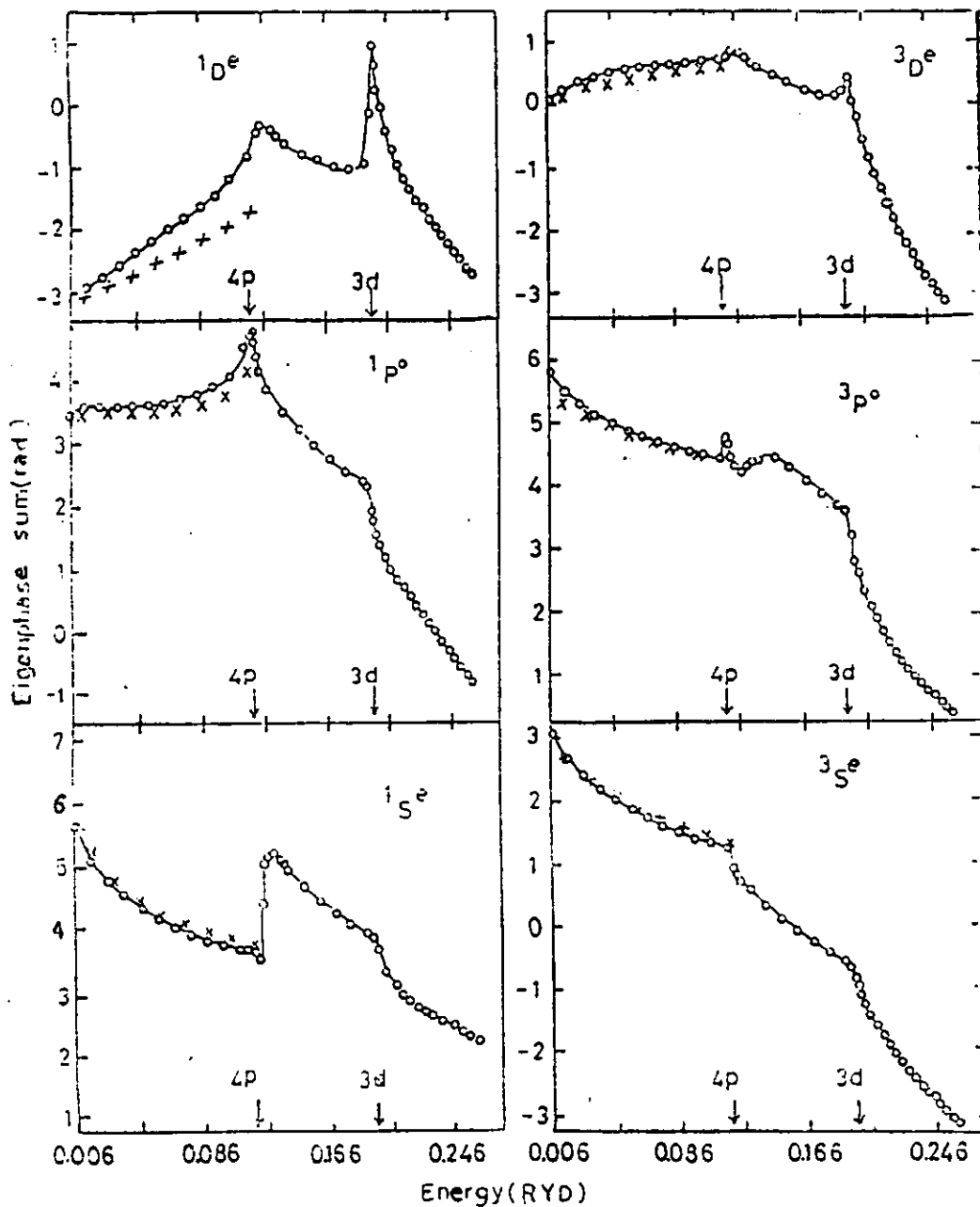


figure (1) Eigenphase sum for singlet and triplet states in electron-potassium scattering; xxx are Karule results.

Delta J. Sci. 15 (3) 1991

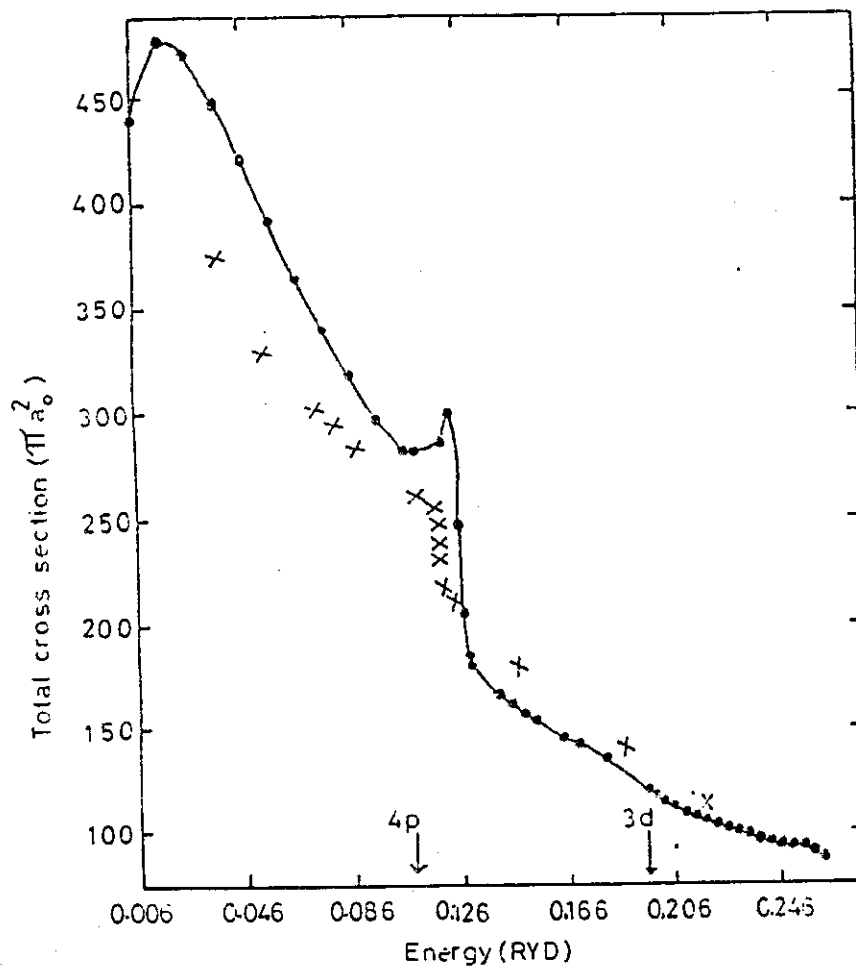


Figure (2) Total cross section for $4s \rightarrow 4s$ transition; xxx are Moore's results.

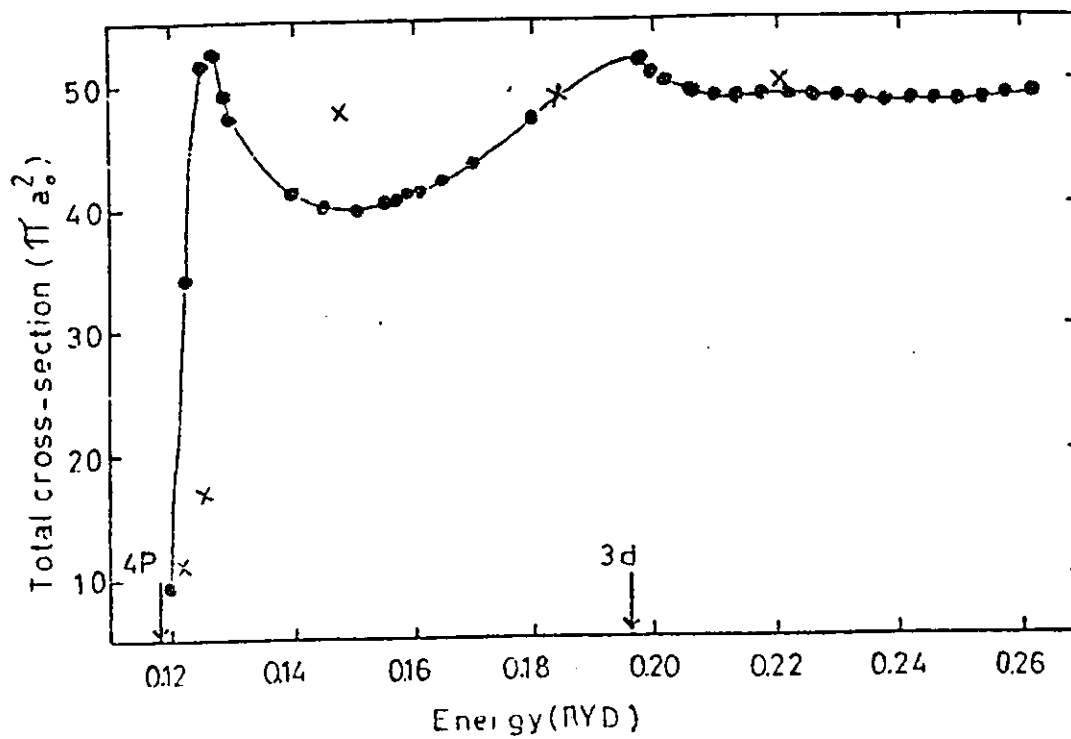


figure (3) AS figure 2 for $4s \rightarrow 4p$ transition.

Delta J. Sci. 15 (3) 1991

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استطارة الالكترونات بواسطة نرات البوتاسيوم عند طاقات منخفضة

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طبقت طريقة المصفوفة - آر لحساب مجموع الاطوار المناسبة ومساحات المقطع الكلية للالكترونات الساقطة على نرات البوتاسيوم بطاقات من صفر حتى ٣٥ الكترون فولت. استخدمت طريقة الحساب الكلى للالكترونات فى الحالات الثلاث (4S, 4p , 3d) لوصف عطية الاستطارة.