T.M. Luke

Corrected oscillator strengths in the neon sequence: $Z \leq 26$

Oscillator strengths for transitions among the $2p^6$, $2p^5 3s$, 3p, 3d levels of ions in the neon sequence have been calculated using the Multi-configuration Optimized Potential Model (MCOPM) (Aashamar et al, 1979). Following this ab initio calculation, many of the levels have been corrected by solving an inverse eigenvalue problem using the observed spectrum as input. This correction may result in improved coefficients for the LS coupled terms that are mixed by spin-orbit and other relativistic contributions in the Breit-Pauli hamiltonian. Results for lifetimes are in reasonable agreement with recent calculations of Fawcett (1984) and others but differences between theory and beam foil experiments remain. Some details follow.

The ab initio MCOPM calculation expands the terms of interest using the following 13 configurations: $2s^2 2p^6$; $2s^2 2p^5 3s$, 3p, 3d, 4s, 4p, 4d; $2s2p^6 3s$, 3p, 3d, 4s, 4p, 4d. In this model, the orbitals are calculated in l-dependent central potentials that are varied to minimize a weighted set of LS coupled term energies. The variational principle leads to integral equations for the potentials which are solved iteratively along with the secular equation for the configuration interaction mixing coefficients. These optimized potentials are used as input to the program SUPERSTRUCTURE of Eissner et al (1974) in which the Breit-Pauli hamiltonian matrix is calculated and diagonalized. Rates for transitions among the resulting fine structure levels are then calculated.

The levels thus obtained frequently have mixing coefficients of comparable size for the terms coupled by relativistic effects and these coefficients can be in significant error if there are small errors in the energies of the non-relativistically calculated terms. These will be apparent if the level spectrum is not correctly reproduced in the calculation.

A scheme has been developed to correct for these errors (Luke,1988). It works as follows: Suppose a given level is predominantly a mixture of four terms (whose wave functions have been obtained in the nonrelativistic CI calculation as mixtures of whatever configurations have been included in the study). The Breit-Pauli hamiltonian matrix can be calculated in the subspace of these four terms and its diagonalization accurately reproduces the spectrum obtained in a full SUPERSTRUCTURE calculation. If this does not however reproduce the observed spectrum, one can invert the problem: Use the observed spectrum as input and calculate a corrected set of diagonal matrix elements that yield this observed spectrum. Corrections to the diagonal elements of the Breit-Pauli hamiltonian used in SUPERSTRUCTURE can then be obtained and hence corrected relativistic term-mixing coefficients and transition rates.

Earlier work has been published for the Neon sequence up to Si V. The present calculations have continued along the sequence with the ions Cl VIII, Ar IX, Ti XIII, Cr XV and Fe XVII selected on account of the availability of sufficient experimental data on the required spectra.

Three outcomes resulted from these calculations. Most commonly, the raw uncorrected calculation using these 13 configurations was quite satisfactory. Corrections had little effect and were not required.

In a number of cases, corrections in the mixing coefficients leading to shifts of the order of 15% in the transition rates occurred.

In a small number of cases the inverse eigenvalue problem has no solution. This may not be surprising: Inverse problems usually lead to difficulties. Among these is the fact that the solution is not unique. The corrected set of diagonal matrix elements results from solving a set of nonlinear algebraic equations and there can be up to n! sets of diagonal matrix elements leading to a given set of eigenvalues. In the present method of solution, the set that evolves smoothly from solving the inverse problem with raw calculated spectrum as input (leading to the known raw calculated solution) to solving with the observed spectrum as input is taken to be the correct solution set.

Occasionally this procedure of numerical continuation doesn't work. At some point in the continuation from raw to observed eigenvalue input, the equations cease to have a solution, in the neighbourhood of earlier

solutions at least. It is likely that the difficulty in these cases is that the equations are especially sensitive to small errors in the off-diagonal elements. This has been found to be true in some cases. Slight perturbations in the off-diagonal elements restore the solution. In the cases where this has been found to occur so far, the mixing coefficients have been rather stable so that the corrections have been very modest anyway. There is no reason to believe this will always be the situation and the remaining cases of non-existence of solution to the inverse eigenvalue problem are still being investigated.

The poster accompanying this abstract gives examples of the various outcomes just described as well as some comparisons with observations and other calculations. Except for some high accuracy laser observations of transition rates in Ne I by Hartmetz and Schmoranzer (1983, 1984), only lifetimes appear to be available from experiment at present and these do not give a very sensitive test of transition rates. Nevertheless some comparisons between theory and experiment are given, illustrating cases of both systematic agreement and discrepancy.

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AUTHOR'S ADDRESS

Department of Applied Mathematics,
University of Western Ontario,
London, Canada.N6A 5B9