Analytical Property of Scattering Matrix: Spectroscopy Phenomena and Sharp Overlapping Autoionization Resonances of Ne^+

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Synopsis With our relativistic eigenchannel R-matrix scenario (i.e., the R-R-Eigen code), the scattering matrices of Ne^+ in the whole energy regions are calculated directly, which correspond to the physics parameters in multi channel quantum defect theory (MQDT). All the energy levels can be obtained with our proposed projected high dimensional quantum-defect graph (symmetrized). On the other hand, based on the analytical continuation property of short-range scattering matrix, the scattering matrices in the whole energy region can be checked/ calibrated systematically against the spectroscopic experimental data on the plots. With this method, the photoionization spectra are calculated with a good agreement with the experiments and are systematically assigned. Hence, important autoionization rates, photoionization rates and so on can be obtained.

In astrophysics studies and the energy researches, an extended atomic data base with sufficiently high precision is required. The conventional R-matrix[1] can be a good candidate to serve the purpose, while the calculation of "infinite" energy levels in discrete energy region as well as overlapping resonances in autoionization region are not trivial. Furthermore, it's difficult to ascertain the accuracies. It also needs a fine energy scanning grid to obtain all the levels and resonances. Based on the analytical continuation properties of scattering matrices, our proposed eigenchannel R-matrix scenario (i.e., the R-R-Eigen code[1]) can solve these difficulties. We will show the merits of this scenario using Ne^+ as an illustration example. In this work, the short range scattering matrices of Ne^+ in both discrete and continuum energy regions for all symmetry blocks (J^p =1/2$^+$, 3/2$^+$ and 5/2$^+$) are calculated with good analytical properties by our R-R-Eigen method directly, which correspond to the physical parameters associated with the multichannel quantum defect theory (MQDT). The corresponding eigenchannel dipole transition matrix elements D_a are also calculated with good analytical properties.

For the Ne^+ case associated with multiple ionization thresholds, i.e., Ne^{2+} ($2p^4\ ^3P_{2,1,0}$, $^1D_2$ and $^1S_0$), we proposed a projected high dimensional quantum-defect graph (symmetrized) as a generalization of Lu-Fano plots for two thresholds to readily check/calibrate the calculated scattering matrices against the experimental energy levels systematically. Based on the analytical continuation properties of short range scattering matrices, the scattering matrices in autoionization energy regions can also be check/ calibrated. Therefore, the calculated resonant photoionization cross sections in the autoionization region are in excellent agreement with the benchmark high resolution experiments conducted at the synchrotron radiation light source[2]. One can be confident that both energy levels and the dynamical processes should be calculated with adequate accuracies comparable to benchmark experiments. Important autoionization rates, photoionization rates and dielectronic rates with enough accuracy can be obtained. It should then satisfy the needs of the astrophysical and energy researches.

References

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