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Relativistic Configuration Interaction Calculation of the Correlation Energies of Highly-Charged Ions

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We are developing a new relativistic configuration interaction (CI) method for calculating the atomic structure of many-electron ions using complete finite basis sets constructed from B spline functions of piecewise polynomials. This method is based on the relativistic no-pair Hamiltonian from quantum electrodynamics (QED). Eigenfuctions of the Hamiltonian are expanded in a basis of configuation state functions constructed from products of one-electron orbitals. Eigenvalues and eigenfunctions of the low-lying states of the ions are then determined by diagonalizing the Hamiltonian matrix which includes the contributions both from the Coulomb and retarded Breit interactions.

The one-electron basis orbitals are B spline solutions of the Dirac equation for an electron in a Coulomb field or a model potential constrained to a finite cavity[1]. The resulting modified Dirac spectrum consists of a finite set of discrete eigenstates which separate cleanly into positive- and negative-energy spectra. The positive-energy branch contains terms that belong to the bound-state spectrum as well as the positive-energy continuum of the unmodified Dirac spectrum. As a result, the use of this B spline basis set in a CI calculation effectively includes interactions with the bound states as well as with the positive-energy continuum. Furthermore, the positive-energy projection operator associated with the relativistic no-pair Hamiltonian can be easily implemented by using only the positive-energy solutions of the modified Dirac equation in the CI calculations.

We have successfully applied this CI method to calculate the term energies of the n=2 triplet states [2] and n=1,2 singlet states of heliumlike ions. In

these calculations, the CI equation leads to a large symmetric eigenvalue problem with dimension of 5000 to 8000. The eigenvalues and eigenfunctions for the lowest few states are determined using the Davidson's method [3].

For the n=2 triplet states of heliumlike ions, mass polarization and QED corrections from Drake's unified method [4] are added to our CI term values for comparisons with experiment. Our term energies are in very good agreement with the results from the relativistic many-body perturbation theory of Johnson and Sapirstein [5]. Discrepancy with Drake's values is due mainly to the neglect of higher-order relativistic corrections in the relativistic no-pair Hamiltonian in Drake's calculations. Our results on fine structure splittings and transition energies agree very well with experiment throughout the whole isoelectronic sequence. For the n=1,2 singlet states of heliumlike ions, QED corrections are calculated with a scheme by Cheng et al. [6] which includes not only the screening but also the relaxation effects. For the Kα x-ray energies, differences between our results and Drake's values for low- and mid-Z ions arise mostly from the relaxation effects in QED corrections which are not included in Drake's calculations. Including relaxation effects in QED corrections improves the agreement between theory and experiment. Residual differences on the order of 0.5 eV for Kr^{34+} are likely due to the higher-order QED corrections not yet considered in any theoretical calculations.

At present, we are extending these new techniques to calculate the n=2 to n=2 transition energies for Be-like heavy ions. Some results for Be-like ions are also discussed.

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